Euler-Rodrigues and Cayley formulas for rotation of elasticity tensors

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Abstract

It is fairly well known that rotation in three dimensions can be expressed as a quadratic in a skew symmetric matrix via the Euler-Rodrigues formula. A generalized Euler-Rodrigues polynomial of degree 2n in a skew symmetric generating matrix is derived for the rotation matrix of tensors of order n. The Euler-Rodrigues formula for rigid body rotation is recovered by n=1. A Cayley form of the n^{th} order rotation tensor is also derived. The representations simplify if there exists some underlying symmetry, as is the case for elasticity tensors such as strain and the fourth order tensor of elastic moduli. A new formula is presented for the transformation of elastic moduli under rotation: as a 21-vector with a rotation matrix given by a polynomial of degree 8. Explicit spectral representations are constructed from three vectors: the axis of rotation and two orthogonal bivectors. The tensor rotation formulae are related to Cartan decomposition of elastic moduli and projection onto hexagonal symmetry.

1 Introduction

Rigid body rotation about an axis \mathbf{p} , $|\mathbf{p}| = 1$, is described by the well known Euler-Rodrigues formula for the rotation matrix as a quadratic in the skew symmetric matrix \mathbf{P} ,

$$P_{ij} = -\epsilon_{ijk} \, p_k,\tag{1}$$

where ϵ_{ijk} is the third order isotropic alternating tensor¹. Thus,

$$\mathbf{Q} = \exp(\theta \mathbf{P}) = \mathbf{I} + \sin \theta \, \mathbf{P} + (1 - \cos \theta) \mathbf{P}^2, \tag{2}$$

where θ is the angle of rotation. Euler first derived this formula although Rodrigues (21) obtained the formula for the composition of successive finite rotations (11; 7). The concise form of the Euler-Rodrigues formula is basically a consequence of the property

$$\mathbf{P}^3 = -\mathbf{P}.\tag{3}$$

¹The summation convention on repeated subscripts is assumed in $(1)_1$ and most elsewhere.

Hence, every term in the power series expansion of $\exp(\theta \mathbf{P})$ is either $\mathbf{P}^{2k} = (-1)^{k+1}\mathbf{P}^2$ or $\mathbf{P}^{2k+1} = (-1)^k\mathbf{P}$, and regrouping yields (2). Rotation about an axis is defined by the proper orthogonal rigid body rotation matrix $\mathbf{Q}(\theta, \mathbf{p}) \in SO(3)$, the special orthogonal group of matrices satisfying²

$$\mathbf{Q}\mathbf{Q}^t = \mathbf{Q}^t\mathbf{Q} = \mathbf{I},\tag{4}$$

and the special property det $\mathbf{Q} = 1$. The generating matrix $\mathbf{P}(\mathbf{p}) \in so(3)$ where so(n) denotes the space of skew symmetric matrices or tensors, usually associated with the Lie algebra of the infinitesimal (or Lie) transformation group defined by rotations in SO(n). Alternatively, SO(3) is isomorphic to so(3) via the Cayley form (4)

$$\mathbf{Q} = (\mathbf{I} + \mathbf{S})(\mathbf{I} - \mathbf{S})^{-1} = (\mathbf{I} - \mathbf{S})^{-1}(\mathbf{I} + \mathbf{S}), \tag{5}$$

where $\mathbf{S} \in so(3)$ follows from (2) as

$$\mathbf{S} = \tanh(\frac{\theta}{2}\mathbf{P}) = \tan\frac{\theta}{2}\mathbf{P}. \tag{6}$$

The first identity is a simple restatement of the definition in (5) with $\mathbf{Q} = \exp(\theta \mathbf{P})$, while the second is a more subtle relation that depends upon (3) and the skew symmetry of \mathbf{P} , and as such is analogous to the Euler-Rodrigues formula.

We are concerned with generalizing these fundamental formulas for rigid body rotation to the rotation matrices associated with \mathbf{Q} but which act on second and higher order tensors in the same way that \mathbf{Q} transforms a vector as $\mathbf{v} \to \mathbf{v}' = \mathbf{Q}^t \mathbf{v}$. If one takes the view that the rotation transforms a set of orthonormal basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$, then the coordinates of a fixed vector $\mathbf{v} = v_1 \mathbf{e}_1 + v_2 \mathbf{e}_2 + v_3 \mathbf{e}_3$ relative to this basis transform according to $(v_1, v_2, v_3) \to (v_1', v_2', v_3')$, where $v_i' = Q_{ij}v_j$. A tensor \mathbb{T} of order (or rank) n has elements, or components relative to a vector basis, $T_{ij...kl}$. Under rotation of the basis vectors by \mathbf{Q} , the elements are transformed by the relations

$$T'_{ij\dots kl} = Q_{ij\dots klpq\dots rs} T_{pq\dots rs}, \tag{7}$$

where $\mathbb{Q} = \mathbb{Q}(\theta, \mathbf{p})$ is a tensor of order 2n formed from n combinations of the underlying rotation,

$$Q_{\underbrace{ij\dots kl}_{p}\underbrace{pq\dots rs}_{p}} \equiv \underbrace{Q_{ip}Q_{jq}\dots Q_{kr}Q_{ls}}_{p}. \tag{8}$$

 \mathbb{Q} is also known as the *n*-th Kronecker power of \mathbb{Q} (18). Lu and Papadopoulos (14) derived a generalized *n*-th order Euler-Rodrigues formula for \mathbb{Q} as a polynomial of degree 2n in the tensor \mathbb{P} , also of order 2n, defined by the sum of n terms

$$P_{ij\dots klpq\dots rs} = P_{ip}\delta_{jq}\dots\delta_{kr}\delta_{ls} + \delta_{ip}P_{jq}\dots\delta_{kr}\delta_{ls} + \dots + \delta_{ip}\delta_{jq}\dots P_{kr}\delta_{ls} + \delta_{ip}\delta_{jq}\dots\delta_{kr}P_{ls}.$$
 (9)

Thus,

$$\mathbb{Q} = \exp(\theta \, \mathbb{P}) = P_{2n}(\theta, \, \mathbb{P}), \tag{10}$$

where

$$P_{2n}(\theta, x) = \sum_{k=-n}^{n} e^{\lambda_k \theta} \prod_{\substack{j=-n\\j\neq k}}^{n} \left(\frac{x - \lambda_j}{\lambda_k - \lambda_j}\right), \quad \text{with } \lambda_k = k i, \quad i = \sqrt{-1}.$$
 (11)

Lu and Papadopoulos' derivation of (11) is summarized in Section 3. The case n = 2 has also been derived in quite different ways by Podio-Guidugli and Virga (20) and by Mehrabadi et al. (16).

 $^{{}^{2}\}mathbf{Q}^{t}$ denotes transpose and **I** is the identity.

The purpose of this paper is twofold. First, to obtain alternative forms of the generalized Euler-Rodrigues formula and of the associated Cayley form. Using general properties of skew symmetric matrices we will show that the n-th order Euler-Rodrigues formula can be expressed in ways which clearly generalize the classical n=1 case. The difference in approach from that of Lu and Papadopoulos (14) can be appreciated by noting that their formula (11) follows from the fact that the eigenvalues of \mathbb{P} are λ_k , $k=-n,\ldots,n$, of eq. (11). The present formulation is based on the more fundamental property that \mathbb{P} has canonical form

$$\mathbb{P} = \mathbb{P}_1 + 2 \, \mathbb{P}_2 + \ldots + n \, \mathbb{P}_n, \tag{12}$$

where \mathbb{P}_j satisfy identities similar to (3), and are mutually orthogonal in the sense of tensor product. This allows us to express $\exp(\theta \mathbb{P})$ and $\tanh(\frac{\theta}{2}\mathbb{P})$ in forms that more clearly generalize (2) and (6). Furthermore, the base tensors \mathbb{P}_j can be expressed in terms of powers of \mathbb{P} , which imply explicit equations for \mathbb{Q} and the related \mathbb{S} . We will derive these equations in Section 3.

The second objective is to derive related results for rotation of tensors in elasticity. The underlying symmetry of the physical tensors, strain, elastic moduli, etc., allow further simplification from the 2n- tensors $\mathbb{Q} \in SO(3^n)$ and $\mathbb{P} \in so(3^n)$, where the nominal dimensionality 3^n assumes no symmetry. Thus, Mehrabadi et al. (16) expressed the rotation tensor associated with strain, n=2, in term of second order tensors in 6-dimensions, significantly reducing the number of components required. By analogy, the rotation matrix for fourth order elastic stiffness tensors is derived here as a second order tensor in 21-dimensions $\widetilde{\mathbf{Q}}(\theta,\mathbf{p}) = \exp\left(\theta\widetilde{P}\right) \in SO(21)$ where $\widetilde{P} \in so(21)$. This provides an alternative to existing methods for calculating elastic moduli under a change of basis, e.g. using Bond transformation matrices (3) or other methods based on representations of the moduli as elements of 6×6 symmetric matrices (16). Viewing the elastic moduli as a 21-vector is the simplest approach for some purposes, such as projection onto particular symmetries (12; 6). In fact, we will see that the generalized Euler-Rodrigues formula leads to a natural method for projecting onto hexagonal symmetry defined by the axis \mathbf{p} , as an explicit expression for the projector appears quite naturally.

The third and final result is a general formulation of the so-called Cartan decomposition (8) of tensor rotation. The action of \mathbf{Q} of (2) on a vector leaves the component parallel to the axis \mathbf{p} unchanged, and the component perpendicular to it rotates through angle θ . The latter decreases the part perpendicular to \mathbf{p} to $\cos\theta$ of its original value, and introduces $\sin\theta$ times the same magnitude but in in a direction orthogonal to both the vector and the axis. This simple geometrical interpretation generalizes for tensors, in that we can identify "components" that remain unchanged, and others that rotate according to $\cos j\theta$, $\sin j\theta$, $j=1,2,\ldots,n$. The components form subspaces that rotate independently of one another, just as the axial and perpendicular components of the vector do for n=1. This is the essence of Cartan decomposition of tensors, see (8) for further details. Our main result is that the components and the subspaces can be easily identified and defined using the properties of \mathbb{P} and \mathbb{Q} that follow from (12).

We begin with a summary of the main findings in Section 2, with general results applicable to tensors of arbitrary order described in Section 3. Further details of the proofs are given in Section 4. Applications to elasticity are described in Section 5 where the 21 dimensional rotation of elastic moduli is derived. Finally, the relation between the generalized Euler-Rodrigues formula and the Cartan decomposition of elasticity tensors is discussed in Section 6.

A note on notation: tensors of order n are denoted \mathbb{P} , \mathbb{Q} , etc. Vectors and matrices in 3D are normally lower and capital boldface, e.g. \mathbf{p} , \mathbf{Q} , while quantities in 6-dimensions are denoted e.g. $\widehat{\mathbf{Q}}$, and in 21-dimensions as \widetilde{Q} .

2 Summary of results

Our principal result is

Theorem 1 The rotation tensor $\mathbb{Q}(\theta, \mathbf{p}) = \exp(\theta \mathbb{P})$ has the form

$$\mathbb{Q} = \mathbb{I} + \sum_{k=1}^{n} \left(\sin k\theta \, \mathbb{P}_k + (1 - \cos k\theta) \, \mathbb{P}_k^2 \right) \tag{13}$$

where \mathbb{P}_k , k = 1, 2, ..., n are mutually orthogonal skew-symmetric tensors that partition \mathbb{P} and have the same basic property as \mathbf{P} in (3),

$$\mathbb{P} = \mathbb{P}_1 + 2 \, \mathbb{P}_2 + \ldots + n \, \mathbb{P}_n, \tag{14a}$$

$$\mathbb{P}_i \, \mathbb{P}_i = \mathbb{P}_i \, \mathbb{P}_i = 0, \quad i \neq j, \tag{14b}$$

$$\mathbb{P}_i^3 = -\mathbb{P}_i. \tag{14c}$$

The Cayley form for \mathbb{Q} is

$$\mathbb{Q} = (\mathbb{I} + \mathbb{S}) (\mathbb{I} - \mathbb{S})^{-1} = (\mathbb{I} - \mathbb{S})^{-1} (\mathbb{I} + \mathbb{S}), \tag{15}$$

where

$$S = \sum_{k=1}^{n} \tan(k\frac{\theta}{2}) \, \mathbb{P}_k \,. \tag{16}$$

The tensors \mathbb{P}_k are uniquely defined by polynomials of \mathbb{P} of degree 2n-1,

$$\mathbb{P}_{k} = p_{n,k}(\mathbb{P}), \quad \text{where} \quad p_{n,k}(x) = \frac{x}{k} \prod_{\substack{j=1\\j \neq k}}^{n} \left(\frac{x^{2} + j^{2}}{j^{2} - k^{2}}\right), \quad 1 \leq k \leq n.$$
 (17)

The polynomial representation $\mathbb{Q} = P_{2n}(\theta, \mathbb{P})$ has several alternative forms, three of which are as follows:

$$P_{2n}(\theta, x) = 1 + \sum_{k=1}^{n} \frac{2(-1)^{k+1}}{(n-k)! (n+k)!} \left[k \sin k\theta \, x + (1 - \cos k\theta) \, x^2 \right] \prod_{\substack{j=1\\ j \neq k}}^{n} (x^2 + j^2)$$
 (18a)

$$=1+\sum_{k=1}^{n}\frac{(2\sin\frac{\theta}{2})^{2k-1}}{k(2k-1)!}\left(k\cos\frac{\theta}{2}x+\sin\frac{\theta}{2}x^{2}\right)\prod_{l=1}^{k-1}(x^{2}+l^{2})$$
(18b)

$$= 1 + \sin \theta \, x \left(1 + \frac{X_1}{1} \left(1 + \frac{X_2}{2} \left(1 + \frac{X_3}{3} (1 + \dots + \frac{X_{n-1}}{n-1}) \right) \right) \right)$$

+
$$(1 - \cos \theta) x^2 \left(1 + \frac{X_1}{2} \left(1 + \frac{X_2}{3} \left(1 + \frac{X_3}{4} \left(1 + \dots + \frac{X_{n-1}}{n}\right)\right)\right)\right),$$
 (18c)

where

$$X_j = (1 - \cos \theta)(x^2 + j^2)/(2j + 1). \tag{19}$$

We note that n = 1, 2, 3, 4 corresponds to rotation of vectors, second, third and fourth order tensors, respectively. All these are covered by considering n = 4 in Theorem 1, for which the series (18c) and (18a) are, respectively,

$$P_8(\theta, x) = 1 + \sin \theta \, x \left(1 + \frac{(1 - \cos \theta)}{1.3} (x^2 + 1) \left[1 + \frac{(1 - \cos \theta)}{2.5} (x^2 + 4) \left(1 + \frac{(1 - \cos \theta)}{3.7} (x^2 + 9) \right) \right] \right)$$

$$+ (1 - \cos \theta) x^{2} \left(1 + \frac{(1 - \cos \theta)}{2.3} (x^{2} + 1) \left[1 + \frac{(1 - \cos \theta)}{3.5} (x^{2} + 4) \left(1 + \frac{(1 - \cos \theta)}{4.7} (x^{2} + 9) \right) \right] \right)$$

$$= 1 + \frac{1}{5!3} \left[\sin \theta x + (1 - \cos \theta) x^{2} \right] (x^{2} + 4) (x^{2} + 9) (x^{2} + 16)$$

$$- \frac{1}{6!} \left[2 \sin 2\theta x + (1 - \cos 2\theta) x^{2} \right] (x^{2} + 1) (x^{2} + 9) (x^{2} + 16)$$

$$+ \frac{2}{7!} \left[3 \sin 3\theta x + (1 - \cos 3\theta) x^{2} \right] (x^{2} + 1) (x^{2} + 4) (x^{2} + 16)$$

$$- \frac{2}{8!} \left[4 \sin 4\theta x + (1 - \cos 4\theta) x^{2} \right] (x^{2} + 1) (x^{2} + 4) (x^{2} + 9) .$$

$$(20)$$

This expression includes all the Euler-Rodrigues type formulas for tensors of order $n \leq 4$, on account of the characteristic polynomial equation for \mathbb{P} of degree 2n + 1,

$$\mathbb{P}(\mathbb{P}^2 + \mathbb{I})(\mathbb{P}^2 + 4\mathbb{I}) \dots (\mathbb{P}^2 + n^2\mathbb{I}) = 0.$$
 (21)

Thus, the last line in (20) vanishes for n = 3, the last two for n = 2, and all but the first line for n = 1, while the terms that remain can be simplified using (21). The formulas for P_{2n} , n = 2 and 3, are

$$P_4(\theta, x) = 1 + \sin \theta x \left(1 + \frac{1}{3} (1 - \cos \theta)(x^2 + 1) \right) + (1 - \cos \theta) x^2 \left(1 + \frac{1}{6} (1 - \cos \theta)(x^2 + 1) \right), \quad (22a)$$

$$P_6(\theta, x) = 1 + \sin \theta x \left(1 + \frac{1}{3} (1 - \cos \theta)(x^2 + 1) \left[1 + \frac{1}{10} (1 - \cos \theta)(x^2 + 4) \right] \right)$$

$$+ (1 - \cos \theta) x^2 \left(1 + \frac{1}{6} (1 - \cos \theta)(x^2 + 1) \left[1 + \frac{1}{15} (1 - \cos \theta)(x^2 + 4) \right] \right). \quad (22b)$$

These identities apply for $n \leq 2$ and $n \leq 3$, respectively, since they reduce to, e.g. the n = 1 formula using (21).

The second main result is a matrix representation for simplified forms of \mathbb{P} and \mathbb{Q} for 4th order elasticity tensors. Although of fourth order, symmetries reduce the maximum number of elements from 3^4 to 21, and hence the moduli can be described by a 21-vector and \mathbb{P} and \mathbb{Q} by 21 × 21 matrices. This reduction in matrix size is similar to the 6×6 representation of Mehrabadi et al. (16) for symmetric second order tensors. The case of third order tensors (n=3) is not discussed here to the same degree of detail as for second and fourth order, but it could be considered in the same manner. The following Theorem provides the matrices for n=1,2,4, corresponding to rotation of vectors, symmetric second order tensors, and fourth order elasticity tensors, respectively.

Theorem 2 The skew-symmetric matrices and the associated rotation matrices defined by the tensors (\mathbb{P}, \mathbb{Q}) for n = 1, 2, 4, are given by (\mathbf{P}, \mathbf{Q}) , $(\widehat{\mathbf{P}}, \widehat{\mathbf{Q}})$ and $(\widetilde{\mathbf{P}}, \widehat{\mathbf{Q}})$, respectively. The $m \times m$, m = 3, 6, 21, skew symmetric generator matrix for each case has the form

$$P = R - R^t, (23)$$

where

$$\mathbf{R} = -\mathbf{X}, \quad \text{for vectors}, \ n = 1,$$
 (24a)

$$\widehat{\mathbf{R}} = \begin{pmatrix} \mathbf{0} & \sqrt{2}\mathbf{Y} \\ \sqrt{2}\mathbf{Z} & \mathbf{X} \end{pmatrix}, \quad \text{for symmetric tensors, } n = 2,$$
 (24b)

$$\widetilde{\mathbf{R}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 2\mathbf{Y} & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{2}\mathbf{Y} & 0 & \sqrt{2}\mathbf{N} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\mathbf{N} & -\sqrt{2}\mathbf{Y} \\ 0 & -\sqrt{2}\mathbf{Z} & 0 & 0 & \mathbf{X} & 0 & -\sqrt{2}\mathbf{X} \\ 0 & \sqrt{2}\mathbf{N} & 2\mathbf{N} & 0 & 0 & \mathbf{X} & 0 \\ 2\mathbf{Z} & 0 & 0 & \mathbf{X} & 0 & 0 & \sqrt{2}\mathbf{X} \\ 0 & 0 & -\sqrt{2}\mathbf{Z} & -\sqrt{2}\mathbf{X} & \sqrt{2}\mathbf{X} & 0 & -\mathbf{X} \end{pmatrix}, \quad \begin{array}{c} \textit{for elasticity} \\ \textit{tensors}, \ n = 4, \\ \end{aligned}$$

with $\mathbf{0} = \mathbf{0}_{3\times 3}$ and

$$\mathbf{X} = \begin{pmatrix} 0 & p_3 & 0 \\ 0 & 0 & p_1 \\ p_2 & 0 & 0 \end{pmatrix}, \quad \mathbf{Y} = \begin{pmatrix} 0 & p_2 & 0 \\ 0 & 0 & p_3 \\ p_1 & 0 & 0 \end{pmatrix}, \quad \mathbf{Z} = \begin{pmatrix} 0 & p_1 & 0 \\ 0 & 0 & p_2 \\ p_3 & 0 & 0 \end{pmatrix}, \quad \mathbf{N} = \begin{pmatrix} p_1 & 0 & 0 \\ 0 & p_2 & 0 \\ 0 & 0 & p_3 \end{pmatrix}. \quad (25)$$

In each case, the Q-matrix is given by Theorem 1, and the tensors acted on by Q are m-vectors which transform like v' = Qv.

The specific form of the 6- and 21-vectors are given in Section 5.

The third and final result identifies subspaces that are closed under rotation:

Theorem 3 The Cartan components of an n-th order tensor \mathbb{T} are defined as

$$\mathbb{T}_0 = \mathbb{M}_0 \, \mathbb{T}, \qquad \mathbb{T}_j \equiv \mathbb{M}_j \, \mathbb{T}, \quad \mathbb{R}_j \equiv \mathbb{P}_j \, \mathbb{T}, \quad j = 1, 2, \dots, n.$$
 (26)

where the n+1 symmetric projection tensors, \mathbb{M}_k , $k=0,1,\ldots,n$, are

$$\mathbb{M}_0 \equiv \mathbb{I} + \mathbb{P}_1^2 + \mathbb{P}_2^2 + \ldots + \mathbb{P}_n^2, \qquad \mathbb{M}_i = -\mathbb{P}_i^2, \quad i = 1, 2, \ldots, n.$$
 (27)

They satisfy, for $0 \le k \le n$ and $1 \le i \le n$,

$$\mathbb{M}_i \mathbb{M}_k = \mathbb{M}_k \mathbb{M}_i = \mathbb{M}_k \mathbb{P}_i = \mathbb{P}_i \mathbb{M}_k = 0, \quad i \neq k, \tag{28a}$$

$$\mathbb{M}_k^2 = \mathbb{M}_k, \qquad \mathbb{M}_i \, \mathbb{P}_i = \mathbb{P}_i \, \mathbb{M}_i = \mathbb{P}_i,$$
 (28b)

$$\mathbb{M}_{k} = m_{n,k}(\mathbb{P}), \qquad m_{n,k}(x) = \frac{(-1)^{k} (2 - \delta_{k0})}{(n-k)!(n+k)!} \prod_{\substack{j=0\\j \neq k}}^{n} (x^{2} + j^{2}).$$
 (28c)

The projection \mathbb{T}_0 along with the n-pairs $\{\mathbb{T}_j, \mathbb{R}_j\}$, j = 1, 2, ..., n define n + 1 subspaces that are closed under rotation:

$$\mathbb{Q}\,\mathbb{T}_0 = \mathbb{T}_0, \qquad \mathbb{Q}\,\mathbb{T}_j = \cos j\theta\,\mathbb{T}_j + \sin j\theta\,\mathbb{R}_j, \qquad \mathbb{Q}\,\mathbb{R}_j = \cos j\theta\,\mathbb{R}_j - \sin j\theta\,\mathbb{T}_j, \qquad j = 1, 2, \dots, n. \tag{29}$$

The meaning will become more apparent by example, as we consider the various cases of tensors of order n = 1, 2, and 4 in Section 6.

3 General theory for tensors

3.1 P's and Q's

The transpose of a 2n-th order tensor is defined by interchanging the first and last n indices. In particular, the skew symmetry of \mathbf{P} and the definition of \mathbb{P} in (9) implies that $\mathbb{P}^t = -\mathbb{P}$. Based on the definitions of \mathbb{Q} in (8) and the properties of the fundamental rotation $\mathbf{Q} \in SO(3)$, \mathbb{Q} of (10) satisfies

$$\frac{\mathrm{d}\,\mathbb{Q}}{\mathrm{d}\theta} = \mathbb{P}\,\mathbb{Q},\tag{30}$$

where the product of two tensors of order 2n is another tensor of order 2n defined by contracting over n indices, $(AB)_{ij...klpq...rs} = A_{ij...klab...cd} B_{ab...cdpq...rs}$. This gives meaning to the representation

$$\mathbb{Q} = e^{\theta \, \mathbb{P}}.\tag{31}$$

Based on the skew symmetry of \mathbb{P} it follows that

$$\mathbb{Q} \mathbb{Q}^t = \mathbb{Q}^t \mathbb{Q} = \mathbb{I}, \text{ where } I_{ij\dots klpq\dots rs} = \overbrace{\delta_{ip}\delta_{jq}\dots\delta_{kr}\delta_{ls}}^n$$
 (32)

The isomorphism between the space of n-th order tensors and a vector space of dimension 3^n implies that $\mathbb{Q} \in SO(3^n)$ and $\mathbb{P} \in so(3^n)$.

The derivation of the main result in Theorem 1 is outlined next using a series of Lemmas. Details of the proof are provided below and in the Appendix.

Lemma 1 For any $N \geq 1$, a given non-zero $N \times N$ skew symmetric matrix B has $2m \leq N$ distinct non-zero eigenvalues of the form $\{\pm ic_1, \pm ic_2, \ldots, \pm ic_m\}$, c_1, \ldots, c_m real, and B has the representation

$$B = c_1 B_1 + c_2 B_2 + \ldots + c_m B_m, (33a)$$

$$B_i B_j = B_j B_i = 0, \quad i \neq j, \tag{33b}$$

$$B_i^3 = -B_i. (33c)$$

Lemma 1 is essentially Theorem 2.2 of Gallier and Xu (9), who also noted the immediate corollary

$$e^{B} = I + \sum_{k=1}^{\infty} \frac{1}{k!} \left(c_{1}B_{1} + c_{2}B_{2} + \dots + c_{m}B_{m} \right)^{k}$$

$$= I + \sum_{k=1}^{\infty} \frac{1}{k!} \left(c_{1}^{k}B_{1}^{k} + c_{2}^{k}B_{2}^{k} + \dots + c_{m}^{k}B_{m}^{k} \right)$$

$$= e^{c_{1}B_{1}} + e^{c_{2}B_{2}} + \dots + e^{c_{m}B_{m}} - (m-1)I$$

$$= I + \sum_{j=1}^{m} \left(\sin c_{j}B_{j} + (1 - \cos c_{j})B_{j}^{2} \right).$$
(34)

Thus, the exponential of any skew symmetric matrix has the form of a sum of Euler-Rodrigues terms.

Lemma 2 The elements of the decomposition of Lemma 1 can be expressed in terms of the matrix B and its eigenvalues by

$$B_j = \frac{B}{c_j} \prod_{\substack{k=1\\k \neq j}}^m \left(\frac{B^2 + c_k^2}{c_k^2 - c_j^2} \right), \tag{35}$$

Equation (35) may be obtained by starting with

$$B(B^{2} + c_{k}^{2}) = \sum_{\substack{j=1\\j\neq k}}^{m} (c_{k}^{2} - c_{j}^{2})c_{j}B_{j},$$
(36)

and iterating until a single B_j remains. Equation (35) in combination with (34) and $B_j^2 = c_j^{-1}BB_j$ implies that e^B can be expressed as a polynomial of degree 2m in B,

$$e^{B} = I + \sum_{j=1}^{m} \left[c_{j} \sin c_{j} B + (1 - \cos c_{j}) B^{2} \right] c_{j}^{-2} \prod_{\substack{k=1\\k \neq j}}^{m} \left(\frac{B^{2} + c_{k}^{2}}{c_{k}^{2} - c_{j}^{2}} \right).$$
 (37)

We are now ready to consider $\exp(\theta \mathbb{P})$.

Lemma 3 The non-zero eigenvalues of the skew symmetric tensor \mathbb{P} defined in eq. (9) are

$$\{i, -i, 2i, -2i, \dots, ni, -ni\}.$$

This follows from Zheng and Spence (23) or Lu and Papadopoulos (14), and is discussed in detail in Section 4. \mathbb{P} therefore satisfies the characteristic equation (21), and has the properties

$$\mathbb{P} = \mathbb{P}_1 + 2 \,\mathbb{P}_2 + \ldots + n \,\mathbb{P}_n,\tag{38a}$$

$$\mathbb{P}_i \, \mathbb{P}_i = \mathbb{P}_i \, \mathbb{P}_i = 0, \quad i \neq j, \tag{38b}$$

$$\mathbb{P}_i^3 = -\mathbb{P}_i. \tag{38c}$$

Equation (38a) is the canonical decomposition of \mathbb{P} into orthogonal components each of which has properties like the fundamental \mathbf{P} in (3), although the subspace associated with \mathbb{P}_i can be multidimensional. The polynomials $p_{n,k}(x)$ of eq. (17) follow from (35), or alternatively,

$$p_{n,k}(x) = \frac{(-1)^{k+1} 2kx}{(n-k)!(n+k)!} \prod_{\substack{j=1\\j\neq k}}^{n} (x^2 + j^2), \quad 1 \le k \le n.$$
 (39)

We will examine the particular form of the \mathbb{P}_i for elasticity tensors of order n=2 and n=4 in Section 5. For now we note the consequence of Lemmas 2 and 3,

$$e^{\theta \mathbb{P}} = \mathbb{I} + \sum_{k=1}^{n} \left[k \sin k\theta \, \mathbb{P} + (1 - \cos k\theta) \, \mathbb{P}^{2} \right] k^{-2} \prod_{\substack{j=1 \ j \neq k}}^{n} \left(\frac{\mathbb{P}^{2} + j^{2} \mathbb{I}}{j^{2} - k^{2}} \right). \tag{40}$$

Together with (31) this implies the first expression (18a) in Theorem 1. The alternative identities (18b) and (18c) are derived in the Appendix.

Lemma 4 \mathbb{Q} may be expressed in Cayley form

$$\mathbb{Q} = (\mathbb{I} + \mathbb{S}) (\mathbb{I} - \mathbb{S})^{-1} = (\mathbb{I} - \mathbb{S})^{-1} (\mathbb{I} + \mathbb{S}), \tag{41}$$

where the 2n-th order skew symmetric tensor \mathbb{S} is

$$S = \tanh(\frac{\theta}{2} \mathbb{P}) = \sum_{k=1}^{n} \tan(k\frac{\theta}{2}) \mathbb{P}_{k}.$$
 (42)

This follows by inverting (41) and using the expression (13) for \mathbb{Q} ,

$$\mathbb{S} = \mathbb{I} - 2(\mathbb{I} + \mathbb{Q})^{-1} = \mathbb{I} - \left[\mathbb{I} + \sum_{k=1}^{n} \frac{1}{2} \left(\sin k\theta \, \mathbb{P}_k + (1 - \cos k\theta) \, \mathbb{P}_k^2\right)\right]^{-1},\tag{43}$$

and then applying the following identity,

$$\left[\mathbb{I} + \sum_{k=1}^{n} \left(a_k \, \mathbb{P}_k + (1 - b_k) \, \mathbb{P}_k^2 \right) \right]^{-1} = \mathbb{I} + \sum_{k=1}^{n} \left(-\frac{a_k}{a_k^2 + b_k^2} \, \mathbb{P}_k + (1 - \frac{b_k}{a_k^2 + b_k^2}) \, \mathbb{P}_k^2 \right). \tag{44}$$

Note that Lemma 4 combined with the obvious result $(42)_1$ implies that, for arbitrary ϕ ,

$$\tanh(\phi \,\mathbb{P}) = \sum_{k=1}^{n} \, \tan(k\phi) \,\mathbb{P}_{k}. \tag{45}$$

This is a far more general statement than the simple partition of (12), and in fact may be shown to be equivalent to eq. (38).

3.2 Equivalence with the Lu and Papadopoulos formula

We now show that (40) agrees with the polynomial of Lu and Papadopoulos (14). They derived eq. (11) directly using Sylvester's interpolation formula (p. 437 of Horn and Johnson (13)). Thus, the function $f(\mathbf{A})$ defined by a power series for a matrix \mathbf{A} that is diagonalizable can be expressed in terms of its distinct eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_r$ as $f(\mathbf{A}) = p(\mathbf{A})$, where p(x) is

$$p(x) = \sum_{i=1}^{r} f(\lambda_i) L_i(x), \qquad L_i(x) = \prod_{\substack{j=1\\j \neq i}}^{r} \left(\frac{x - \lambda_j}{\lambda_i - \lambda_j}\right). \tag{46}$$

 $L_i(x)$ are the Legendre interpolation polynomials and p(x) is the unique polynomial of degree r-1 with the property $p(\lambda_i) = f(\lambda_i)$. Equation (11) follows from the explicit form of the spectrum of \mathbb{P} . The right member of (11) can be rewritten in the following form by combining the terms $e^{\pm ik\theta}$,

$$P_{2n}(\theta, x) = \frac{1}{(n!)^2} \prod_{j=1}^{n} (x^2 + j^2) + \sum_{k=1}^{n} \frac{2(-1)^{k+1}}{(n-k)! (n+k)!} \left(k \sin k\theta \, x - \cos k\theta \, x^2 \right) \prod_{\substack{j=1\\j \neq k}}^{n} (x^2 + j^2) \,. \tag{47}$$

The first term on the right hand side can be written in a form which agrees with (18a) by considering the partial fraction expansion of $1/\Lambda$ where

$$\Lambda(x) = \prod_{k=1}^{n} (x^2 + k^2). \tag{48}$$

Thus, as may be checked by comparing residues, for example,

$$\frac{1}{\Lambda} = \sum_{k=1}^{n} \frac{2(-1)^{k+1}}{(n-k)! (n+k)!} \frac{k^2}{x^2 + k^2}$$

$$= \sum_{k=1}^{n} \frac{2(-1)^{k+1}}{(n-k)! (n+k)!} - \sum_{k=1}^{n} \frac{2(-1)^{k+1}}{(n-k)! (n+k)!} \frac{x^2}{x^2 + k^2}.$$
(49)

The first term in the right member is $1/\Lambda(0) = 1/(n!)^2$. Multiplying by $\Lambda(x)/\Lambda(0)$ implies the identity

$$\frac{1}{(n!)^2} \prod_{j=1}^n (x^2 + j^2) = 1 + \sum_{k=1}^n \frac{2x^2(-1)^{k+1}}{(n-k)! (n+k)!} \prod_{\substack{j=1\\j \neq k}}^n (x^2 + j^2), \tag{50}$$

which combined with (47) allows us recover the form (18a). This transformation from the interpolating polynomial (11) to the alternative forms in eq. (18) is rigorous but it does not capture the physical basis of the latter. We will find the identity (50) useful in Section 6.

4 Eigenvalues of \mathbb{P} and application to second order tensors

The key quantity in the polynomial representation of \mathbb{Q} is the set of distinct non-zero eigenvalues of \mathbb{P} , Lemma 3. We prove this by construction, starting with the case of n = 1.

4.1 Rotation of vectors, n = 1

Let $\{p, q, r\}$ form an orthonormal triad of vectors, then the eigenvalues and eigenvectors of **P** are as follows

eigenvalue eigenvector
$$\begin{array}{ccc}
0 & \mathbf{p} \\
\pm i & \mathbf{v}_{\pm} \equiv \frac{1}{\sqrt{2}} (i\mathbf{q} \pm \mathbf{r})
\end{array} \tag{51}$$

These may be checked using the properties of the third order alternating tensor. Thus, $P_{ij}q_j = r_i$, $P_{ij}r_j = -q_i$, implying $\mathbf{P}\mathbf{v}_{\pm} = \pm i\mathbf{v}_{\pm}$. Hence, the spectral representation of \mathbf{P} is

$$\mathbf{P} = i\mathbf{v}_{+}\mathbf{v}_{+}^{*} - i\mathbf{v}_{-}\mathbf{v}_{-}^{*}, \tag{52}$$

where * denotes complex conjugate. It also denotes transpose if we view eq. (52) in vector/matrix format. We can also think of this as a tensorial representation in which terms such as $\mathbf{v}_-\mathbf{v}_-^*$ stand for the Hermitian dyadic $\mathbf{v}_- \otimes \mathbf{v}_-^*$, however, for simplicity of notation we do not use dyadic notation further but take the view that dyadics are obvious from the context.

The bivectors (5) \mathbf{v}_{\pm} , together with the axis \mathbf{p} , will serve as the building blocks for spectral representations of \mathbb{P} for n > 1.

Referring to eq. (38), we see that $\mathbb{P} = \mathbb{P}_1$ in this case. Equation (52) allows us to evaluate powers and other functions of **P**. Thus, in turn,

$$\mathbf{P}^2 = -\mathbf{v}_+ \mathbf{v}_+^* - \mathbf{v}_- \mathbf{v}_-^* \,, \tag{53a}$$

$$\mathbf{P}^2 + \mathbf{I} = \mathbf{p}\mathbf{p},\tag{53b}$$

$$\mathbf{P}(\mathbf{P}^2 + \mathbf{I}) = 0,\tag{53c}$$

from which the characteristic equation (3) follows.

4.2 Rotation of second order tensors, n = 2

In this case the tensors \mathbb{P} and \mathbb{Q} are fourth order with, see eq. (9),

$$P_{ijkl} = P_{ik}\delta_{jl} + \delta_{ik}P_{jl}. (54)$$

Equation (17) implies

$$\mathbb{P}_1 = \mathbb{P}(\mathbb{P}^2 + 4)/3, \qquad \mathbb{P}_2 = -\mathbb{P}(\mathbb{P}^2 + 1)/6, \tag{55}$$

which clearly satisfy the decomposition (38a)

$$\mathbb{P} = \mathbb{P}_1 + 2\,\mathbb{P}_2. \tag{56}$$

The skew symmetric tensor \mathbb{S} of (16) may be expressed

$$S = \left(\frac{4}{3}\tan\frac{\theta}{2} - \frac{1}{6}\tan\frac{3\theta}{2}\right)\mathbb{P} + \left(\frac{1}{3}\tan\frac{\theta}{2} - \frac{1}{6}\tan\frac{3\theta}{2}\right)\mathbb{P}^3.$$
 (57)

Consider the product of the second order tensor (dyad) $\mathbf{p}\mathbf{v}_{\pm}$ with \mathbb{P} . Thus, $\mathbb{P}\mathbf{p}\mathbf{v}_{\pm} = \pm i\mathbf{p}\mathbf{v}_{\pm}$ which together with $\mathbb{P}\mathbf{v}_{\pm}\mathbf{p} = \pm i\mathbf{v}_{\pm}\mathbf{p}$ yields 4 eigenvectors, two pairs with eigenvalue i and -i. The dyadics $\mathbf{v}_{\pm}\mathbf{v}_{\pm}$ are also eigenvectors and have eigenvalues $\pm 2i$. The remaining 3 eigenvectors of \mathbb{P} are null vectors which can be identified as $\mathbf{p}\mathbf{p}$, $\mathbf{v}_{+}\mathbf{v}_{-}$ and $\mathbf{v}_{-}\mathbf{v}_{+}$. This completes the $3^{n} = 9$ eigenvalues and eigenvectors, and shows that the non-zero eigenvalues are $\{i(2), -i(2), 2i, -2i\}$ where the number in parenthesis indicates the multiplicity. The tensors \mathbb{P}_{1} and \mathbb{P}_{2} can be expressed explicitly in terms of the eigenvectors,

$$\mathbb{P}_1 = i\mathbf{p}\mathbf{v}_+\mathbf{p}\mathbf{v}_+^* + i\mathbf{v}_+\mathbf{p}\mathbf{v}_+^*\mathbf{p} - i\mathbf{p}\mathbf{v}_-\mathbf{p}\mathbf{v}_-^* - i\mathbf{v}_-\mathbf{p}\mathbf{v}_-^*\mathbf{p}, \qquad \mathbb{P}_2 = i\mathbf{v}_+\mathbf{v}_+^*\mathbf{v}_+^* - i\mathbf{v}_-\mathbf{v}_-^*\mathbf{v}_-^*. \quad (58)$$

It is straightforward to show that these satisfy the conditions (38).

We note in passing that zero eigenvalues correspond to tensors of order n with rotational or transversely isotropic symmetry about the \mathbf{p} axis. This demonstrates that there are three second order basis tensors for transversely isotropic symmetry. We will discuss this aspect in greater detail in Section 6 in the context of elasticity tensors.

Both \mathbb{P} and \mathbb{Q} correspond to $3^n \times 3^n$ or 9×9 matrices, which we denote P and Q, with the precise form dependent on how we choose to represent second order tensors as 9-vectors. To be specific, let T_{ij} be the components of a second order tensor (not symmetric in general), and define the 9-vector

$$T = (T_{11}, T_{22}, T_{33}, T_{23}, T_{31}, T_{12}, T_{32}, T_{13}, T_{21})^{t}.$$

$$(59)$$

The form of P follows from the expansion (7) for small θ , or from (9), as

$$P = \begin{pmatrix} 0 & 0 & 0 & 0 & p_2 & -p_3 & 0 & p_2 & -p_3 \\ 0 & 0 & 0 & -p_1 & 0 & p_3 & -p_1 & 0 & p_3 \\ 0 & 0 & 0 & p_1 & -p_2 & 0 & p_1 & -p_2 & 0 \\ 0 & p_1 & -p_1 & 0 & 0 & 0 & 0 & p_3 & -p_2 \\ -p_2 & 0 & p_2 & 0 & 0 & 0 & -p_3 & 0 & p_1 \\ p_3 & -p_3 & 0 & 0 & 0 & 0 & p_2 & -p_1 & 0 \\ 0 & p_1 & -p_1 & 0 & p_3 & -p_2 & 0 & 0 & 0 \\ -p_2 & 0 & p_2 & -p_3 & 0 & p_1 & 0 & 0 & 0 \\ p_3 & -p_3 & 0 & p_2 & -p_1 & 0 & 0 & 0 & 0 \end{pmatrix}.$$
 (60)

This can be written in block matrix form using the X, Y, Z matrices defined in eq. (25),

$$P = R - R^t$$
, where $R = \begin{pmatrix} \mathbf{0} & \mathbf{Y} & \mathbf{Y} \\ \mathbf{Z} & \mathbf{0} & \mathbf{X} \\ \mathbf{Z} & \mathbf{X} & \mathbf{0} \end{pmatrix}$. (61)

Note that this partition of the skew symmetric matrix is not unique.

4.3 Tensors of arbitrary order $n \ge 2$

The example of second order tensors shows that the three eigenvectors $\{\mathbf{p}, \mathbf{v}_+, \mathbf{v}_-\}$ of the fundamental matrix \mathbf{P} define all $3^n = 9$ eigenvectors of \mathbb{P} . This generalizes to arbitrary $n \geq 2$ by generation of all possible n-tensors formed from the tensor outer product of $\{\mathbf{p}, \mathbf{v}_+, \mathbf{v}_-\}$. For any n, consider the product \mathbb{P} with the n-tensor

$$v_{+} = \underbrace{\mathbf{v}_{+}\mathbf{v}_{+}\dots\mathbf{v}_{+}}_{n} . \tag{62}$$

Each of the n terms of \mathbb{P} in (9) contributes $+iv_+$ with the result $\mathbb{P}v_+ = ni\,v_+$. Similarly, defining v_- implies $\mathbb{P}v_- = -ni\,v_-$, from which it is clear that there are no other eigenvectors with eigenvalues $\pm ni$. Thus, the final component in the decomposition (38a) is

$$\mathbb{P}_n = i \, v_+ v_+^* - i \, v_- v_-^* \,. \tag{63}$$

Next consider the *n n*-th order tensors that are combinations of (n-1) times \mathbf{v}_+ with a single \mathbf{p} , e.g.

$$v = \mathbf{p} \underbrace{\mathbf{v}_{+} \mathbf{v}_{+} \dots \mathbf{v}_{+}}_{n-1} . \tag{64}$$

The action of \mathbb{P} is $\mathbb{P}v = (n-1)iv$, and so there are 2n eigenvectors with eigenvalues $\pm (n-1)i$ which can be combined together to form the component \mathbb{P}_{n-1} , as in eq. $(58)_1$ for n=2. Eigenvalues (n-2)i are obtained by combining \mathbf{p} twice with \mathbf{v}_+ (n-2) times, but also come from n-tensors formed by a single \mathbf{v}_- with (n-1) times \mathbf{v}_+ . Enumeration yields a total of n(n+1) eigenvectors associated with \mathbb{P}_{n-2} . By recursion, it is clear that the number of eigenvectors with eigenvalues ki equals the number of ways n elements chosen from $\{-1,0,1\}$ sum to $-n \leq k \leq n$, or equivalently, the coefficient of x^k in the expansion of $(1+x+x^{-1})^n$,

$$(1+x+x^{-1})^n = \sum_{k=-n}^n \binom{n}{k}_2 x^k.$$
 (65)

The numbers $\binom{n}{k}_2$ are trinomial coefficients (not to be confused with q-multinomial coefficients (1) with q=3) and can be expressed (2)

$$\binom{n}{k}_2 = \sum_{j=0}^n \binom{n}{2j+k} \binom{2j+k}{j},\tag{66}$$

where $\binom{n}{j} = n!/(j!(n-j)!)$ are binomial coefficients. The main point for the present purpose is that

$$\sum_{k=-n}^{n} \binom{n}{k}_2 = 3^n, \tag{67}$$

which is a consequence of (65) with x = 1. It is clear from this process that the entire set of 3^n eigenvectors has been obtained and there are no other candidates for eigenvalue of \mathbb{P} . The precise form of the eigenvectors is unimportant because the Euler-Rodrigues type formulas (18) depend only on the set of distinct non-zero eigenvalues. However, the eigenvectors do play a role in setting up matrix representations of \mathbb{P} for specific values of n, and in particular for tensors with symmetries, as discussed in Section 5.

5 Applications to elasticity

We first demonstrate that the underlying symmetry of second and fourth order tensors in elasticity implies symmetries in the rotation tensors which reduces the number of independent elements in the latter.

5.1 Rotation of symmetric second and fourth order tensors

We consider second and fourth order tensors such as the elastic strain ε (n=2) and the elastic stiffness tensor \mathbb{C} (n=4) with elements ε_{ij} and C_{ijkl} . They transform as $\varepsilon_{ij} \to \varepsilon'_{ij}$ and $C_{ijkl} \to C'_{ijkl}$,

$$\varepsilon'_{ij} = Q_{ijpq}\varepsilon_{pq} \qquad C'_{ijkl} = Q_{ijklpqrs}C_{pqrs},$$
 (68)

where the rotation tensors follow from the general definition (8) as

$$Q_{ijpq} = Q_{ip}Q_{jq}, Q_{ijklpqrs} = Q_{ijpq}Q_{klrs}. (69)$$

The strain and stiffness tensors possess physical symmetries which reduce the number of independent elements that need to be considered,

$$\varepsilon_{ij} = \varepsilon_{ji}, \qquad C_{ijkl} = C_{jikl} = C_{ijlk}, \qquad C_{ijkl} = C_{klij}.$$
(70)

In short, the number of independent elements of ε is reduced from 9 to 6, and of \mathbb{C} from 81 to 21. Accordingly, we may define variants of Q_{ijkl} and $Q_{ijklpqrs}$ with a reduced number of elements that reflect the underlying symmetries of elasticity. Thus, the transformation rules can be expressed in the alternative forms

$$\varepsilon'_{ij} = \overline{Q}_{ijpq} \varepsilon_{pq}, \qquad C'_{ijkl} = \overline{Q}_{ijklpqrs} C_{pqrs},$$
 (71)

where the elements of the symmetrized 4th and 8th order $\overline{\mathbb{Q}}$ tensors are

$$\overline{Q}_{ijpq} = \frac{1}{2} (Q_{ijpq} + Q_{ijqp}), \tag{72a}$$

$$\overline{Q}_{ijklpqrs} = \frac{1}{2} \left(\overline{Q}_{ijpq} \overline{Q}_{klrs} + \overline{Q}_{ijrs} \overline{Q}_{klpq} \right). \tag{72b}$$

Alternatively, they can be expressed in terms of the fundamental $\mathbf{Q} \in SO(3)$,

$$\overline{Q}_{ijpq} = \frac{1}{2} (Q_{ip}Q_{jq} + Q_{iq}Q_{jp}), \tag{73a}$$

$$\overline{Q}_{ijklpqrs} = \frac{1}{8} \left(Q_{ip} Q_{jq} Q_{kr} Q_{ls} + Q_{ip} Q_{jq} Q_{ks} Q_{lr} + Q_{iq} Q_{jp} Q_{kr} Q_{ls} + Q_{iq} Q_{jp} Q_{ks} Q_{lr} + Q_{ir} Q_{js} Q_{kp} Q_{lq} + Q_{ir} Q_{js} Q_{kq} Q_{lp} + Q_{is} Q_{jr} Q_{kp} Q_{lq} + Q_{is} Q_{jr} Q_{kq} Q_{lp} \right).$$
(73b)

Using the identity (32), we have

$$\overline{Q}_{ijpq}\overline{Q}_{klpq} = \frac{1}{2} (I_{ijkl} + I_{ijlk}) = \overline{I}_{ijkl} \equiv \frac{1}{2} (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{74}$$

which is the fourth order isotropic identity tensor, i.e. the fourth order tensor with the property $s = \overline{\mathbb{I}}s$ for all symmetric second order tensors s. Similarly,

$$\overline{Q}_{ijklabcd}\overline{Q}_{pqrsabcd} = \frac{1}{2} \left(\overline{I}_{ijpq} \overline{I}_{klrs} + \overline{I}_{ijrs} \overline{I}_{klpq} \right) \equiv \overline{I}_{ijklpqrs}. \tag{75}$$

This is the 8th order isotropic tensor with the property $\mathbb{C} = \overline{\mathbb{I}} \mathbb{C}$ for all 4th order elasticity tensors. In summary, the symmetrized rotation tensors for strain and elastic moduli are orthogonal in the sense that $\overline{\mathbb{Q}} \overline{\mathbb{Q}}^t = \overline{\mathbb{I}}$, and are therefore elements of SO(6) and SO(21), respectively.

The (symmetrized) rotation tensor for strain displays the following symmetries

$$\overline{Q}_{ijpq} = \overline{Q}_{jipq} = \overline{Q}_{ijqp}. \tag{76}$$

Introducing the Voigt indices, which are capital suffices taking the values 1, 2, ..., 6 according to

$$I = 1, 2, 3, 4, 5, 6 \qquad \Leftrightarrow \qquad ij = 11, 22, 33, 23, 31, 12, \tag{77}$$

then (76) implies that the elements \overline{Q}_{ijpq} can be represented by \overline{Q}_{IJ} . Similarly, the elements of the 8th order tensor $\overline{Q}_{ijklpqrs}$ can be represented as \overline{Q}_{IJKL} , which satisfy the symmetries

$$\overline{Q}_{IJKL} = \overline{Q}_{JIKL} = \overline{Q}_{IJLK}.$$
(78)

The pairs of indices IJ and KL each represent 21 independent values, suggesting the introduction of a new type of suffix which ranges from 1, 2, ..., 21. Thus,

$$\mathcal{I} = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21$$

$$\Leftrightarrow IJ = 11, 22, 33, 23, 31, 12, 44, 55, 66, 14, 25, 36, 34, 15, 26, 24, 35, 16, 56, 64, 45. \tag{79}$$

Hence the elements $\overline{Q}_{ijklpqrs}$ can be represented uniquely by the $(21)^2$ elements $\overline{Q}_{\mathcal{I}\mathcal{J}}$. The elements of the symmetrized rotations \overline{Q}_{IJ} and $\overline{Q}_{\mathcal{I}\mathcal{J}}$ have reduced dimensions, 6 and 21 respectively, but do not yet represent the matrix elements of 6- and 21-dimensional tensors. That step is completed next, after which we can define the associated skew symmetric generating matrices and return to the generalized Euler-Rodrigues formulas for 6- and 21-dimensional matrices.

5.2 Six dimensional representation

We now use the isomorphism between second order tensors in three dimensions, such as the strain ε , and six dimensional vectors according to $\varepsilon \to \hat{\varepsilon}$ with elements $\hat{\varepsilon}_I$, I = 1, 2, ..., 6. Similarly, fourth order elasticity tensors in three dimensions are isomorphic with second order positive definite symmetric tensors in six dimensions $\hat{\mathbf{C}}$ with elements \hat{c}_{IJ} (15). Let $\{\varepsilon\}$ be the 6-vector with elements ε_I , I = 1, 2, ..., 6, and [C] the 6×6 Voigt matrix of elastic moduli, i.e. with elements c_{IJ} . The associated 6-dimensional vector and tensor are

$$\hat{\boldsymbol{\varepsilon}} = \mathbf{T}\{\boldsymbol{\varepsilon}\}, \qquad \widehat{\mathbf{C}} = \mathbf{T}[C]\mathbf{T}, \quad \text{where } \mathbf{T} \equiv \operatorname{diag}(1, 1, 1, \sqrt{2}, \sqrt{2}, \sqrt{2}).$$
 (80)

Explicitly,

$$\hat{\boldsymbol{\varepsilon}} = \begin{pmatrix} \hat{\varepsilon}_{1} \\ \hat{\varepsilon}_{2} \\ \hat{\varepsilon}_{3} \\ \hat{\varepsilon}_{4} \\ \hat{\varepsilon}_{5} \\ \hat{\varepsilon}_{6} \end{pmatrix} = \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2}\varepsilon_{23} \\ \sqrt{2}\varepsilon_{31} \\ \sqrt{2}\varepsilon_{12} \end{pmatrix}, \qquad \hat{\mathbf{C}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 2^{\frac{1}{2}}c_{14} & 2^{\frac{1}{2}}c_{15} & 2^{\frac{1}{2}}c_{16} \\ c_{22} & c_{23} & 2^{\frac{1}{2}}c_{24} & 2^{\frac{1}{2}}c_{25} & 2^{\frac{1}{2}}c_{26} \\ c_{33} & 2^{\frac{1}{2}}c_{34} & 2^{\frac{1}{2}}c_{35} & 2^{\frac{1}{2}}c_{36} \\ c_{24} & 2c_{45} & 2c_{46} \\ c_{25} & c_{266} \end{pmatrix}.$$

$$(81)$$

The $\sqrt{2}$ terms ensure that products and norms are preserved, e.g. $C_{ijkl}C_{ijkl}=\operatorname{tr}\widehat{\mathbf{C}}^t\widehat{\mathbf{C}}$.

The six-dimensional version of the fourth order tensor \overline{Q}_{ijkl} is $\widehat{\mathbf{Q}} \in SO(6)$, introduced by Mehrabadi et al. (16), see also (19). It may be defined in the same manner as $\widehat{\mathbf{Q}} = \mathbf{S}[\overline{Q}]\mathbf{S}$ where $[\overline{Q}]$ is the matrix of Voigt elements. Thus, $\widehat{\mathbf{Q}}\widehat{\mathbf{Q}}^t = \widehat{\mathbf{Q}}^t\widehat{\mathbf{Q}} = \widehat{\mathbf{I}}$, where $\widehat{\mathbf{I}} = \text{diag}(1, 1, 1, 1, 1, 1)$. It can be expressed $\widehat{\mathbf{Q}}(\mathbf{p}, \theta) = \exp(\theta\widehat{\mathbf{P}})$, and hence is given by the n = 2 Euler-Rodrigues formula (22) for the skew symmetric $\widehat{\mathbf{P}}(\mathbf{p}) \in so(6)$,

$$\widehat{\mathbf{P}} = \begin{pmatrix} 0 & 0 & 0 & 0 & \sqrt{2}p_2 & -\sqrt{2}p_3 \\ 0 & 0 & 0 & -\sqrt{2}p_1 & 0 & \sqrt{2}p_3 \\ 0 & 0 & 0 & \sqrt{2}p_1 & -\sqrt{2}p_2 & 0 \\ 0 & \sqrt{2}p_1 & -\sqrt{2}p_1 & 0 & p_3 & -p_2 \\ -\sqrt{2}p_2 & 0 & \sqrt{2}p_2 & -p_3 & 0 & p_1 \\ \sqrt{2}p_3 & -\sqrt{2}p_3 & 0 & p_2 & -p_1 & 0 \end{pmatrix}, \tag{82}$$

or in terms of the block matrices defined in (25)

$$\widehat{\mathbf{P}} = \widehat{\mathbf{R}} - \widehat{\mathbf{R}}^t, \qquad \widehat{\mathbf{R}} = \begin{pmatrix} \mathbf{0} & \sqrt{2}\mathbf{Y} \\ \sqrt{2}\mathbf{Z} & \mathbf{X} \end{pmatrix}.$$
 (83)

It is useful to compare $\widehat{\mathbf{P}}$ with the 9×9 matrix for rotation of general second order tensors, eqs. (60) and (61). The reduced dimensions and the $\sqrt{2}$ terms are a consequence of the underlying symmetry of the tensors that are being rotated. Vectors and tensors transform as $\hat{\boldsymbol{\varepsilon}} \to \hat{\boldsymbol{\varepsilon}}'$ and $\widehat{\mathbf{C}} \to \widehat{\mathbf{C}}'$ where

$$\hat{\varepsilon}' = \widehat{\mathbf{Q}}\,\hat{\varepsilon}, \qquad \widehat{\mathbf{C}}' = \widehat{\mathbf{Q}}\widehat{\mathbf{C}}\widehat{\mathbf{Q}}^t.$$
 (84)

The eigenvalues and orthonormal eigenvectors of $\hat{\mathbf{P}}$ are as follows

eigenvalue eigenvector dyadic
$$0 \qquad \hat{\mathbf{i}} \qquad \frac{1}{\sqrt{3}}\mathbf{I}$$

$$0 \qquad \hat{\mathbf{p}}_{d} \qquad \sqrt{\frac{3}{2}}(\mathbf{p}\mathbf{p} - \frac{1}{3}\mathbf{I})$$

$$\pm i \qquad \hat{\mathbf{u}}_{\pm} \qquad \frac{1}{\sqrt{2}}(\mathbf{p}\mathbf{v}_{\pm} + \mathbf{v}_{\pm}\mathbf{p})$$

$$\pm 2i \qquad \hat{\mathbf{v}}_{\pm} \qquad \mathbf{v}_{\pm}\mathbf{v}_{\pm}$$
(85)

where \mathbf{v}_{\pm} are defined in (51) and

$$\hat{\mathbf{i}} \equiv \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \hat{\mathbf{p}}_{d} \equiv \sqrt{\frac{3}{2}} \begin{pmatrix} p_{1}^{2} - \frac{1}{3} \\ p_{2}^{2} - \frac{1}{3} \\ p_{3}^{2} - \frac{1}{3} \\ \sqrt{2} p_{2} p_{3} \\ \sqrt{2} p_{3} p_{1} \\ \sqrt{2} p_{1} p_{2} \end{pmatrix}, \quad \hat{\mathbf{u}}_{\pm} \equiv \begin{pmatrix} \sqrt{2} p_{1} v_{\pm,1} \\ \sqrt{2} p_{2} v_{\pm,2} \\ \sqrt{2} p_{3} v_{\pm,3} \\ p_{2} v_{\pm,3} + p_{3} v_{\pm,2} \\ p_{3} v_{\pm,1} + p_{1} v_{\pm,3} \\ p_{1} v_{\pm,2} + p_{2} v_{\pm,1} \end{pmatrix}, \quad \hat{\mathbf{v}}_{\pm} \equiv \begin{pmatrix} v_{\pm,1}^{2} \\ v_{\pm,2}^{2} \\ v_{\pm,3}^{2} \\ \sqrt{2} v_{\pm,2} v_{\pm,3} \\ \sqrt{2} v_{\pm,3} v_{\pm,1} \\ \sqrt{2} v_{\pm,1} v_{\pm,2} \end{pmatrix}. \quad (86)$$

The right column in (85) shows the second order tensors corresponding to the eigenvectors in dyadic form. The eigenvectors are orthonormal, i.e. of unit magnitude and mutually orthogonal. The unit 6-vectors $\hat{\bf i}$ and $\hat{\bf p}_{\rm d}$ correspond to the hydrostatic and deviatoric parts of $\bf pp$, respectively. The double multiplicity of the zero eigenvalue means that any 6-vector of the form $a\hat{\bf p}_{\rm d}+b\hat{\bf i}$ is a null vector of $\hat{\bf P}$, including $\sqrt{\frac{2}{3}}\hat{\bf p}_{\rm d}+\frac{1}{\sqrt{3}}\hat{\bf i}$ which is the six-vector for the dyad $\bf pp$.

The canonical decomposition of the generating matrix $\widehat{\mathbf{P}} \in so(6)$ is therefore

$$\hat{\mathbf{P}} = \hat{\mathbf{P}}_1 + 2\hat{\mathbf{P}}_2, \qquad \hat{\mathbf{P}}_1 = i\hat{\mathbf{u}}_+\hat{\mathbf{u}}_+^* - i\hat{\mathbf{u}}_-\hat{\mathbf{u}}_-^*, \quad \hat{\mathbf{P}}_2 = i\hat{\mathbf{v}}_+\hat{\mathbf{v}}_+^* - i\hat{\mathbf{v}}_-\hat{\mathbf{v}}_-^*.$$
 (87)

The associated fourth order tensor $\overline{\mathbb{P}}$, which is the symmetrized version of \mathbb{P} in eq. (56), is

$$\overline{\mathbb{P}} = \overline{\mathbb{P}}_1 + 2\overline{\mathbb{P}}_2, \qquad \overline{\mathbb{P}}_1 = \sum_{\pm} \frac{i}{2} (\mathbf{p} \mathbf{v}_{\pm} + \mathbf{v}_{\pm} \mathbf{p}) (\mathbf{p} \mathbf{v}_{\pm}^* + \mathbf{v}_{\pm}^* \mathbf{p}), \quad \overline{\mathbb{P}}_2 = \sum_{\pm} \pm i \, \mathbf{v}_{\pm} \mathbf{v}_{\pm}^* \mathbf{v}_{\pm}^*. \tag{88}$$

The representation (87) allows us to compute powers of $\widehat{\mathbf{P}}$, and using the spectral decomposition of the identity

$$\hat{\mathbf{I}} = \hat{\mathbf{i}}\hat{\mathbf{i}}^t + \hat{\mathbf{p}}_{d}\hat{\mathbf{p}}_{d}^t + \hat{\mathbf{u}}_{+}\hat{\mathbf{u}}_{+}^* + \hat{\mathbf{u}}_{-}\hat{\mathbf{u}}_{-}^* + \hat{\mathbf{v}}_{+}\hat{\mathbf{v}}_{+}^* + \hat{\mathbf{v}}_{-}\hat{\mathbf{v}}_{-}^*,$$
(89)

the characteristic equation (16) follows:

$$\widehat{\mathbf{P}}(\widehat{\mathbf{P}}^2 + \widehat{\mathbf{I}})(\widehat{\mathbf{P}}^2 + 4\widehat{\mathbf{I}}) = 0. \tag{90}$$

5.3 21 dimensional representation

Vectors and matrices in 21-dimensions are denoted by a tilde. Thus, the 21-dimensional vector of elastic moduli is $\tilde{\mathbf{c}}$ with elements $\tilde{c}_{\mathcal{I}}$, $\mathcal{I} = 1, 2, \ldots, 21$. Similarly, vectors corresponding to the fourth order tensors $\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}$ and $\frac{1}{2}(\mathbf{A} \otimes \mathbf{B} + \mathbf{B} \otimes \mathbf{A})$ are $\tilde{\boldsymbol{\varepsilon}}$ and $\tilde{\mathbf{v}}$, that is

$$\begin{array}{cccc}
4^{th} \text{ order, n=3} & 2^{nd} \text{ order, n=6} & \text{vector, n=21} \\
\mathbb{C} & \widehat{\mathbf{C}} & \widetilde{\mathbf{c}} \\
\boldsymbol{\varepsilon}\boldsymbol{\varepsilon} & \hat{\boldsymbol{\varepsilon}}\hat{\boldsymbol{\varepsilon}}^{t} & \widetilde{\boldsymbol{\varepsilon}} \\
\frac{1}{2}(\mathbf{A} \otimes \mathbf{B} + \mathbf{B} \otimes \mathbf{A}) & \frac{1}{2}(\hat{\mathbf{a}}\hat{\mathbf{b}}^{t} + \hat{\mathbf{b}}\hat{\mathbf{a}}^{t}) & \widetilde{\mathbf{v}}
\end{array} \tag{91}$$

The 21 elements follow from the indexing scheme (79) and are defined by

$$\tilde{\mathbf{c}} = \begin{pmatrix} \tilde{c}_1 \\ \tilde{c}_2 \\ \tilde{c}_3 \\ \tilde{c}_4 \\ \tilde{c}_4 \\ \tilde{c}_5 \\ \tilde{c}_5 \\ \tilde{c}_6 \\ \tilde{c}_{11} \\ \tilde{c}_{22} \\ \tilde{c}_5 \\ \tilde{c}_{12} \\ \tilde{c}_{23} \\ \tilde{c}_{44} \\ \tilde{c}_{52} \\ \tilde{c}_{23} \\ \tilde{c}_{5} \\ \tilde{c}_{6} \\ \tilde{c}_{7} \\ \tilde{c}_{2c_{13}} \\ \tilde{c}_{6} \\ \tilde{c}_{7} \\ \tilde{c}_{2c_{13}} \\ \tilde{c}_{8} \\ \tilde{c}_{2c_{13}} \\ \tilde{c}_{6} \\ \tilde{c}_{7} \\ \tilde{c}_{2c_{14}} \\ \tilde{c}_{8} \\ \tilde{c}_{2c_{5}} \\ \tilde{c}_{5} \\ \tilde{c}_{9} \\ \tilde{c}_{2c_{6}} \\ \tilde{c}_{66} \\ \tilde{c}_{2c_{14}} \\ \tilde{c}_{8} \\ \tilde{c}_{2c_{5}} \\ \tilde{c}_{66} \\ \tilde{c}_{2c_{14}} \\ \tilde{c}_{8} \\ \tilde{c}_{2c_{5}} \\ \tilde{c}_{9} \\ \tilde{c}_{2c_{6}} \\ \tilde{c}_{10} \\ \tilde{c}_{11} \\ \tilde{c}_{22} \\ \tilde{c}_{3} \\ \tilde{c}_{4} \\ \tilde{c}_{8} \\ \tilde{c}_{2c_{13}} \\ \tilde{c}_{5} \\ \tilde{c}_{9} \\ \tilde{c}_{2c_{6}} \\ \tilde{c}_{66} \\ \tilde{c}_{2c_{14}} \\ \tilde{c}_{11} \\ \tilde{c}_{2c_{23}} \\ \tilde{c}_{13} \\ \tilde{c}_{14} \\ \tilde{c}_{2c_{25}} \\ \tilde{c}_{234} \\ \tilde{c}_{14} \\ \tilde{c}_{2c_{25}} \\ \tilde{c}_{266} \\ \tilde{c}_{23} \\ \tilde{c}_{236} \\ \tilde{c}_{13} \\ \tilde{c}_{14} \\ \tilde{c}_{2c_{15}} \\ \tilde{c}_{15} \\ \tilde{c}_{2c_{26}} \\ \tilde{c}_{26} \\ \tilde{c}_{27} \\ \tilde{c}_{26} \\ \tilde{c}_{27} \\ \tilde$$

Alternatively,

$$\tilde{\mathbf{c}} = \widetilde{\mathbf{T}}\{c\}, \text{ etc.},$$
(93)

where $\{c\}$ is the 21×1 array with elements $c_{\mathcal{I}}$, and $\widetilde{\mathbf{T}}$ is the the 21×21 diagonal with block structure

$$\widetilde{\mathbf{T}} = \operatorname{diag} \left(\mathbf{I} \sqrt{2} \mathbf{I} \ 2 \mathbf{I} \right). \tag{94}$$

For instance, the elastic energy density $W = \frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}$ is given by the vector inner product

$$W = \frac{1}{2} \, \widetilde{\mathbf{c}}^t \widetilde{\mathbf{c}} \,, \tag{95}$$

where $\tilde{\boldsymbol{\varepsilon}}$ is the 21-vector associated with strain (92).

5.3.1 The 21-dimensional rotation matrix

Vectors in 21-dimensions transform as $\tilde{\mathbf{c}} \to \tilde{\mathbf{c}}' = \widetilde{\mathbf{Q}} \, \tilde{\mathbf{c}}$ where $\widetilde{\mathbf{Q}} \in SO(21)$ satisfies $\widetilde{\mathbf{Q}} \widetilde{\mathbf{Q}}^t = \widetilde{\mathbf{Q}}^t \widetilde{\mathbf{Q}} = \widetilde{\mathbf{I}}$, and $\widetilde{\mathbf{I}}$ is the identity, $\widetilde{I}_{\mathcal{I}\mathcal{J}} = \delta_{\mathcal{I}\mathcal{J}}$. The rotation matrix $\widetilde{\mathbf{Q}}$ can be expressed

$$\widetilde{\mathbf{Q}}(\mathbf{p}, \theta) = e^{\theta \widetilde{\mathbf{P}}},\tag{96}$$

where $\widetilde{\mathbf{P}}(\mathbf{p}) \in so(21)$ follows from the general definition (9) applied to elasticity tensors, i.e. (73b). Thus,

$$\widetilde{\mathbf{P}} = \widetilde{\mathbf{T}}[\overline{P}]\widetilde{\mathbf{T}}, \qquad \widetilde{\mathbf{Q}} = \widetilde{\mathbf{T}}[\overline{Q}]\widetilde{\mathbf{T}}$$
 (97)

(100t)

(100u)

where $[\overline{P}]$, $[\overline{Q}]$ are the 21×21 array with elements $\overline{P}_{\mathcal{I}\mathcal{J}}$, $\overline{Q}_{\mathcal{I}\mathcal{J}}$. We take a slightly different approach, and derive the elements of $\widetilde{\mathbf{P}}$ using the expansion of $\widetilde{\mathbf{Q}}$ for small θ directly. Define the rotational derivative of the moduli as

$$\dot{c}_{ijkl} = \frac{dc'_{ijkl}}{d\theta} \bigg|_{\theta=0} .$$

$$\dot{\widehat{\mathbf{C}}} = \widehat{\mathbf{P}}\widehat{\mathbf{C}} + \widehat{\mathbf{C}}\widehat{\mathbf{P}}^t ,$$
(98)

Using $(84)_2$ for instance, gives

$$\dot{\widehat{\mathbf{C}}} = \widehat{\mathbf{P}}\widehat{\mathbf{C}} + \widehat{\mathbf{C}}\widehat{\mathbf{P}}^t, \tag{99}$$

from which we obtain

$$\begin{array}{llll} \dot{c}_{11} = 4c_{15}p_2 - 4c_{16}p_3 \,, & (100a) \\ \dot{c}_{22} = -4c_{24}p_1 + 4c_{26}p_3 \,, & (100b) \\ \dot{c}_{33} = 4c_{34}p_1 - 4c_{35}p_2 \,, & (100c) \\ \dot{c}_{23} = 2(c_{24} - c_{34})p_1 - 2c_{25}p_2 + 2c_{36}p_3 \,, & (100e) \\ \dot{c}_{13} = 2c_{14}p_1 + 2(c_{35} - c_{15})p_2 - 2c_{36}p_3 \,, & (100e) \\ \dot{c}_{12} = -2c_{14}p_1 + 2c_{25}p_2 + 2(c_{16} - c_{26})p_3 \,, & (100f) \\ \dot{c}_{44} = 2(c_{24} - c_{34})p_1 - 2c_{46}p_2 + 2c_{45}p_3 \,, & (100g) \\ \dot{c}_{55} = 2c_{56}p_1 + 2(c_{35} - c_{15})p_2 - 2c_{45}p_3 \,, & (100h) \\ \dot{c}_{66} = -2c_{56}p_1 + 2c_{46}p_2 + 2(c_{16} - c_{26})p_3 \,, & (100i) \\ \dot{c}_{14} = (c_{12} - c_{13})p_1 - (c_{16} - 2c_{45})p_2 + (c_{15} - 2c_{46})p_3 \,, & (100i) \\ \dot{c}_{25} = (c_{26} - 2c_{45})p_1 + (c_{23} - c_{12})p_2 - (c_{24} - 2c_{56})p_3 \,, & (100l) \\ \dot{c}_{36} = -(c_{35} - 2c_{46})p_1 + (c_{34} - 2c_{56})p_2 + (c_{13} - c_{23})p_3 \,, & (100l) \\ \dot{c}_{34} = -(c_{33} - c_{23} - 2c_{44})p_1 - (c_{36} + 2c_{45})p_2 + c_{35}p_3 \,, & (100m) \\ \dot{c}_{15} = c_{16}p_1 - (c_{11} - c_{13} - 2c_{55})p_2 - (c_{14} + 2c_{56})p_3 \,, & (100m) \\ \dot{c}_{26} = -(c_{25} + 2c_{46})p_1 + c_{24}p_2 - (c_{22} - c_{12} - 2c_{66})p_3 \,, & (100o) \\ \dot{c}_{24} = (c_{22} - c_{23} - 2c_{44})p_1 - c_{26}p_2 + (c_{25} + 2c_{46})p_3 \,, & (100p) \\ \dot{c}_{35} = (c_{36} + 2c_{45})p_1 + (c_{33} - c_{13} - 2c_{55})p_2 - c_{34}p_3 \,, & (100p) \\ \dot{c}_{35} = (c_{36} + 2c_{45})p_1 + (c_{33} - c_{13} - 2c_{55})p_2 - c_{34}p_3 \,, & (100p) \\ \dot{c}_{56} = (c_{66} - c_{55})p_1 + (c_{14} + 2c_{56})p_2 + (c_{11} - c_{12} - 2c_{66})p_3 \,, & (100p) \\ \dot{c}_{56} = (c_{66} - c_{55})p_1 + (c_{36} - c_{16} + c_{45})p_2 - (c_{25} - c_{15} + c_{46})p_3 \,, & (100r) \\ \dot{c}_{56} = (c_{66} - c_{55})p_1 + (c_{36} - c_{16} + c_{45})p_2 - (c_{25} - c_{15} + c_{46})p_3 \,, & (100r) \\ \dot{c}_{56} = (c_{66} - c_{55})p_1 + (c_{36} - c_{16} + c_{45})p_2 - (c_{25} - c_{15} + c_{46})p_3 \,, & (100r) \\ \dot{c}_{56} = (c_{66} - c_{55})p_1 + (c_{36} - c_{16} + c_{45})p_2 - (c_{25} - c_{15} + c_{46})p_3 \,, & (100s) \\ \dot{c}_{56} = (c_{56} - c_{55})p_1 + (c_{36} -$$

The elements of $\widetilde{\mathbf{P}}$ can be read off from this and are given in Table 1. The 21 × 21 format can be simplified to a 7×7 array of block elements, comprising combinations of the 3×3 zero matrix 0 and the 3×3 matrices defined in (25). Thus,

 $\dot{c}_{46} = -(c_{36} - c_{26} + c_{45})p_1 + (c_{44} - c_{66})p_2 + (c_{14} - c_{24} + c_{56})p_3$

 $\dot{c}_{45} = (c_{25} - c_{35} + c_{46})p_1 - (c_{14} - c_{34} + c_{56})p_2 + (c_{55} - c_{44})p_3$.

$$\widetilde{\mathbf{P}} = \widetilde{\mathbf{R}} - \widetilde{\mathbf{R}}^{t}, \quad \text{where} \quad \widetilde{\mathbf{R}} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 2\mathbf{Y} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & -\sqrt{2}\mathbf{Y} & \mathbf{0} & \sqrt{2}\mathbf{N} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 2\mathbf{N} & -\sqrt{2}\mathbf{Y} \\ \mathbf{0} & -\sqrt{2}\mathbf{Z} & \mathbf{0} & \mathbf{0} & \mathbf{X} & \mathbf{0} & -\sqrt{2}\mathbf{X} \\ \mathbf{0} & \sqrt{2}\mathbf{N} & 2\mathbf{N} & \mathbf{0} & \mathbf{0} & \mathbf{X} & \mathbf{0} \\ 2\mathbf{Z} & \mathbf{0} & \mathbf{0} & \mathbf{X} & \mathbf{0} & \mathbf{0} & \sqrt{2}\mathbf{X} \\ \mathbf{0} & \mathbf{0} & -\sqrt{2}\mathbf{Z} & -\sqrt{2}\mathbf{X} & \sqrt{2}\mathbf{X} & \mathbf{0} & -\mathbf{X} \end{pmatrix} . \quad (101)$$

Equation (24) shows that the rotation matrices in three, six and 21 dimensions can be simplified using the fundamental 3×3 matrices $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ and \mathbf{N} . The partition of a skew symmetric matrix in this way is not unique, but it simplifies the calculation and numerical implementation. These matrices satisfy several identities,

$$\mathbf{XX}^t + \mathbf{YY}^t + \mathbf{ZZ}^t = \mathbf{I}, \tag{102a}$$

$$\mathbf{X}^t \mathbf{X} = \mathbf{Y} \mathbf{Y}^t, \quad \mathbf{Y}^t \mathbf{Y} = \mathbf{Z} \mathbf{Z}^t, \quad \mathbf{Z}^t \mathbf{Z} = \mathbf{X} \mathbf{X}^t,$$
 (102b)

$$\mathbf{X}^t \mathbf{Y} = \mathbf{Y} \mathbf{Z}^t, \quad \mathbf{Y}^t \mathbf{Z} = \mathbf{Z} \mathbf{X}^t, \quad \mathbf{Z}^t \mathbf{X} = \mathbf{X} \mathbf{Y}^t,$$
 (102c)

$$\|\mathbf{N}\| = \|\mathbf{X}\| = \|\mathbf{Y}\| = \|\mathbf{Z}\| = 1,\tag{102d}$$

where the norm is $||u|| = \sqrt{\operatorname{tr} u^t u}$.

We find that the eigenvalues of $\widetilde{\mathbf{P}}$ are 0(5), i(3), -i(3), 2i(3), -2i(3), 3i, -3i, 4i, -4i, where the number in parenthesis is the multiplicity. The associated orthonormal eigenvectors of $\widetilde{\mathbf{P}}$ are

eigenvalue	eigenvector	6-dyadic	
0	$\widetilde{\mathbf{v}}_{0a}$	$\hat{f i}\hat{f i}^t$	
0	$\widetilde{\mathbf{v}}_{0b}$	$rac{3}{2}\hat{\mathbf{p}}_{\mathrm{d}}\hat{\mathbf{p}}_{\mathrm{d}}^{t}$	
0	$\widetilde{\mathbf{v}}_{0c}$	$rac{\sqrt{3}}{2}(\hat{\mathbf{i}}\hat{\mathbf{p}}_{\mathrm{d}}^{t}+\hat{\mathbf{p}}_{\mathrm{d}}\hat{\mathbf{i}}^{t})$	
0	$\widetilde{\mathbf{v}}_{0d}$	$rac{1}{\sqrt{2}}(\hat{\mathbf{u}}\hat{\mathbf{u}}_+^t+\hat{\mathbf{u}}_+\hat{\mathbf{u}}^t)$	
0	$\widetilde{\mathbf{v}}_{0e}$	$rac{\hat{\mathbf{v}}_{-}^{2}}{\sqrt{2}}(\hat{\mathbf{v}}_{-}\hat{\mathbf{v}}_{+}^{t}+\hat{\mathbf{v}}_{+}\hat{\mathbf{v}}_{-}^{t})$	
$\pm i$	$\widetilde{\mathbf{v}}_{1a\pm}$	$rac{1}{\sqrt{2}}(\hat{\mathbf{i}}\hat{\mathbf{u}}_{\pm}^t+\hat{\mathbf{u}}_{\pm}\hat{\mathbf{i}}^t)$	(103)
$\pm i$	$\widetilde{\mathbf{v}}_{1b\pm}$	$rac{\sqrt{3}}{2}(\hat{\mathbf{p}}_{\mathrm{d}}\hat{\mathbf{u}}_{\pm}^{t}+\hat{\mathbf{u}}_{\pm}\hat{\mathbf{p}}_{\mathrm{d}}^{t})$, ,
$\pm i$	$\widetilde{\mathbf{v}}_{1c\pm}$	$rac{1}{\sqrt{2}}(\hat{\mathbf{v}}_{\pm}\hat{\mathbf{u}}_{\mp}^t+\hat{\mathbf{u}}_{\mp}\hat{\mathbf{v}}_{\pm}^t)$	
$\pm 2i$	$\widetilde{\mathbf{v}}_{2a\pm}$	$\hat{\mathbf{u}}_{\pm}\hat{\mathbf{u}}_{\pm}^{t}$	
$\pm 2i$	$\widetilde{\mathbf{v}}_{2b\pm}$	$rac{1}{\sqrt{2}}(\hat{\mathbf{i}}\hat{\mathbf{v}}_{\pm}^t+\hat{\mathbf{v}}_{\pm}\hat{\mathbf{i}}^t)$	
$\pm 2i$	$\widetilde{\mathbf{v}}_{2c\pm}$	$rac{\sqrt{3}}{2}(\hat{\mathbf{p}}_{\mathrm{d}}\hat{\mathbf{v}}_{\pm}^{t}+\hat{\mathbf{v}}_{\pm}\hat{\mathbf{p}}_{\mathrm{d}}^{t})$	
$\pm 3i$	$\widetilde{\mathbf{v}}_{3\pm}$	$rac{1}{\sqrt{2}}(\hat{\mathbf{u}}_{\pm}\hat{\mathbf{v}}_{\pm}^t+\hat{\mathbf{v}}_{\pm}\hat{\mathbf{u}}_{\pm}^t)$	
$\pm 4i$	$\widetilde{\mathbf{v}}_{4\pm}$	$\hat{\mathbf{v}}_{\pm}\hat{\mathbf{v}}_{\pm}^{t}$	

Apart from the last two, which have unit multiplicity, these are not unique. For instance, different combinations of the eigenvectors with multiplicity greater than one could be used instead. We also note from their definitions in eqs. (51) and (85) that

$$\mathbf{v}_{\pm}^{*} = -\mathbf{v}_{\mp}, \qquad \hat{\mathbf{u}}_{\pm}^{*} = -\hat{\mathbf{u}}_{\mp}, \qquad \hat{\mathbf{v}}_{\pm}^{*} = \hat{\mathbf{v}}_{\mp}.$$
 (104)

Hence, the five null vectors of $\widetilde{\mathbf{P}}$ in (103) are real. $\widetilde{\mathbf{P}}$ can be expressed in terms of the remaining 16 eigenvectors as

$$\widetilde{\mathbf{P}} = \widetilde{\mathbf{P}}_1 + 2\widetilde{\mathbf{P}}_2 + 3\widetilde{\mathbf{P}}_3 + 4\widetilde{\mathbf{P}}_4,\tag{105}$$

where

$$\widetilde{\mathbf{P}}_{j} = \sum_{\pm} \pm i \sum_{x=a,b,c} \widetilde{\mathbf{v}}_{jx\pm} \widetilde{\mathbf{v}}_{jx\pm}^{*}, \quad j = 1, 2; \qquad \qquad \widetilde{\mathbf{P}}_{j} = \widetilde{\mathbf{v}}_{j\pm} \widetilde{\mathbf{v}}_{j\pm}^{*}, \quad j = 3, 4.$$
(106)

The identity is

$$\widetilde{\mathbf{I}} = \sum_{x=a,b,c,d,e} \widetilde{\mathbf{v}}_{0x} \widetilde{\mathbf{v}}_{0x} + \sum_{\pm} \left(\sum_{x=a,b,c} \left(\widetilde{\mathbf{v}}_{1x\pm} \widetilde{\mathbf{v}}_{1x\pm}^* + \widetilde{\mathbf{v}}_{2x\pm} \widetilde{\mathbf{v}}_{2x\pm}^* \right) + \widetilde{\mathbf{v}}_{3\pm} \widetilde{\mathbf{v}}_{3\pm}^* + \widetilde{\mathbf{v}}_{4\pm} \widetilde{\mathbf{v}}_{4\pm}^* \right).$$
(107)

It is straightforward to demonstrate using these expressions that $\widetilde{\mathbf{P}}$ satisfies

$$\widetilde{\mathbf{P}}\left(\widetilde{\mathbf{P}}^{2}+1\right)\left(\widetilde{\mathbf{P}}^{2}+4\right)\left(\widetilde{\mathbf{P}}^{2}+9\right)\left(\widetilde{\mathbf{P}}^{2}+16\right)=0,\tag{108}$$

which is the characteristic equation for 2n-th order P tensors, eq. (21).

6 Projection onto TI symmetry and Cartan decomposition

It has been mentioned in passing that null vectors of \mathbb{P} and its particular realizations for elasticity tensors correspond to tensors with transversely isotropic symmetry. These are defined as tensors invariant under the action of the group SO(2) associated with rotation about the axis \mathbf{p} . We conclude by making this connection more specific, and relating the theory for the rotation of tensors to the Cartan decomposition, which is introduced below.

6.1 Cartan decomposition

Referring to Theorem 3, the expansion of the projector \mathbb{M}_k defined in eq. (27) as an even polynomial of degree 2n in \mathbb{P} , i.e. of degree n in \mathbb{P}^2 , follows from eqs. (39) and (50) and the identity $\mathbb{P}_k^2 = k^{-1} \mathbb{P} \mathbb{P}_k$. Note that the \mathbb{M}_k tensors partition the identity

$$\mathbb{I} = \mathbb{M}_0 + \mathbb{M}_1 + \ldots + \mathbb{M}_n. \tag{109}$$

Starting with M_0 we have

$$\mathbb{P}\,\mathbb{M}_0 = \,\mathbb{M}_0\,\mathbb{P} = 0,\tag{110}$$

indicating that \mathbb{M}_0 is the linear projection operator onto the null space of \mathbb{P} . In order to examine the remaining n projectors, note that the rotation can be expressed

$$\mathbb{Q} = \mathbb{M}_0 + \sum_{j=1}^n \left(\cos j\theta \, \mathbb{M}_j + \sin j\theta \, \mathbb{P}_j \right). \tag{111}$$

The action of \mathbb{Q} on an n-th order tensor \mathbb{T} , the rotation of \mathbb{T} , can therefore be described as

$$\mathbb{QT} = \mathbb{T}_0 + \sum_{j=1}^n \left(\cos j\theta \, \mathbb{T}_j + \sin j\theta \, \mathbb{R}_j\right), \tag{112}$$

where \mathbb{T}_0 and \mathbb{T}_j , \mathbb{R}_j , $j = 1, 2, \ldots, n$ are defined by (26). We note that \mathbb{R}_j may be expressed

$$\mathbb{R}_j = \mathbb{P}_j \, \mathbb{T}_j = \frac{1}{j} \, \mathbb{P} \, \mathbb{T}_j, \quad j = 1, 2, \dots, n.$$
 (113)

Also, \mathbb{T}_0 is the component of \mathbb{T} in the null space of \mathbb{P} , i.e. the transversely isotropic part of \mathbb{T} . Equation (112) show that \mathbb{T}_0 and the pairs \mathbb{T}_j , \mathbb{R}_j , $j=1,2,\ldots,n$, rotate separately, forming distinct subspaces, and hence proving Theorem 3.

6.2 Application to elasticity tensors

The projection operators are now illustrated with particular application to tensors of low order and elasticity tensors, starting with the simplest case: rotation of vectors.

6.2.1 Vectors, n=1

If n = 1, we have $\mathbb{T} = \mathbf{P}$ of eq. (1), and hence

$$\mathbf{M}_0 = \mathbf{p}\mathbf{p}, \qquad \mathbf{M}_1 = \mathbf{I} - \mathbf{p}\mathbf{p}. \tag{114}$$

Also, $\mathbb{T} \to \mathbf{t}$, an arbitrary vector, and the decomposition (112) and (26) is

$$\mathbf{Qt} = (\mathbf{t} \cdot \mathbf{p})\mathbf{p} + \cos\theta \left[\mathbf{t} - (\mathbf{t} \cdot \mathbf{p})\mathbf{p}\right] + \sin\theta \,\,\mathbf{p} \times \mathbf{t}. \tag{115}$$

Thus, we identify $\mathbf{t}_0 = \mathbf{M}_0 \mathbf{t}$ as the component of the vector parallel to the axis of rotation, $\mathbf{t}_1 = \mathbf{M}_1 \mathbf{t}$ as the orthogonal complement, and $\mathbf{r}_1 = \mathbf{P}_1 \mathbf{t}$ is the rotation of \mathbf{t}_1 about the axis by $\pi/2$.

6.2.2 Second order tensors, n=2

For n=2, we have \mathbb{P}_1 , \mathbb{P}_2 given in (55) and

$$\mathbb{M}_0 = (\mathbb{P}^2 + 1)(\mathbb{P}^2 + 4)/4, \qquad \mathbb{M}_1 = -\mathbb{P}^2(\mathbb{P}^2 + 4)/3, \qquad \mathbb{M}_2 = \mathbb{P}^2(\mathbb{P}^2 + 1)/12.$$
 (116)

The dimensions of the subspaces are \mathbb{T}_0 , 3; \mathbb{T}_1 , 2, ; \mathbb{R}_1 , 2; \mathbb{T}_2 , 1, ; \mathbb{R}_2 , 1.

For symmetric second order tensors the projectors $\widehat{\mathbf{M}}_0$, $\widehat{\mathbf{M}}_1$ and $\widehat{\mathbf{M}}_2$ have the same form as in (116) in terms of $\widehat{\mathbf{P}}$, and may also be expressed in terms of the fundamental vectors introduced earlier. Thus, using (87) and (89),

$$\widehat{\mathbf{M}}_{0} = \frac{1}{4} (\widehat{\mathbf{P}}^{2} + \widehat{\mathbf{I}}) (\widehat{\mathbf{P}}^{2} + 4\widehat{\mathbf{I}}) = \hat{\mathbf{i}}\hat{\mathbf{i}}^{t} + \hat{\mathbf{p}}_{d}\hat{\mathbf{p}}_{d}^{t}, \qquad \widehat{\mathbf{M}}_{1} = \hat{\mathbf{u}}_{+}\hat{\mathbf{u}}_{+}^{*} + \hat{\mathbf{u}}_{-}\hat{\mathbf{u}}_{-}^{*}, \qquad \widehat{\mathbf{M}}_{2} = \hat{\mathbf{v}}_{+}\hat{\mathbf{v}}_{+}^{*} + \hat{\mathbf{v}}_{-}\hat{\mathbf{v}}_{-}^{*}.$$
(117)

Using these and $\widehat{\mathbf{P}}_1$, $\widehat{\mathbf{P}}_2$ from (87), it follows that the subspace associated with $\widehat{\mathbf{M}}_0$ is two dimensional, while $\widehat{\mathbf{M}}_1^{(1)}$, $\widehat{\mathbf{M}}_1^{(2)}$, $\widehat{\mathbf{M}}_2^{(1)}$, and $\widehat{\mathbf{M}}_2^{(2)}$ have dimension one. This Cartan decomposition of the 6-dimensional space Sym agrees with a different approach by Forte and Vianello (8). Alternatively, using (117) and the dyadics in (85), it follows that

$$\mathbb{M}_0 = \mathbf{pppp} + \frac{1}{2}(\mathbf{I} - \mathbf{pp})(\mathbf{I} - \mathbf{pp}), \tag{118a}$$

$$\mathbb{M}_1 = \frac{1}{2}(\mathbf{p}\mathbf{q} + \mathbf{q}\mathbf{p})(\mathbf{p}\mathbf{q} + \mathbf{q}\mathbf{p}) + \frac{1}{2}(\mathbf{p}\mathbf{r} + \mathbf{r}\mathbf{p})(\mathbf{p}\mathbf{r} + \mathbf{r}\mathbf{p}), \tag{118b}$$

$$\mathbb{M}_2 = \frac{1}{2}(\mathbf{q}\mathbf{q} - \mathbf{r}\mathbf{r})(\mathbf{q}\mathbf{q} - \mathbf{r}\mathbf{r}) + \frac{1}{2}(\mathbf{q}\mathbf{r} + \mathbf{r}\mathbf{q})(\mathbf{q}\mathbf{r} + \mathbf{r}\mathbf{q}). \tag{118c}$$

The action of \mathbb{M}_0 on a second order symmetric tensor is

$$\mathbb{M}_0 \mathbf{T} = \mathbf{T}_0 = T_{\parallel} \mathbf{p} \mathbf{p} + T_{\perp} (\mathbf{I} - \mathbf{p} \mathbf{p}), \tag{119}$$

where $T_{\parallel} = \mathbf{T} : \mathbf{pp}$ and $T_{\perp} = \frac{1}{2}(\operatorname{tr} \mathbf{T} - \mathbf{T} : \mathbf{pp})$. It is clear that \mathbf{T}_0 is unchanged under rotation about \mathbf{p} . Similarly, $\mathbb{M}_1 \mathbf{T}$ transforms as a vector under rotation, hence the suffix 1, while $\mathbb{M}_2 \mathbf{T}$ transforms as a second order tensor with elements confined to the plane orthogonal to the axis of rotation.

Let $\mathbf{p} = \mathbf{e}_3$, then using (117)₁ or the simpler (118a) yields

$$\hat{\mathbf{T}}_{0} = \widehat{\mathbf{M}}_{0}(\mathbf{e}_{3})\hat{\mathbf{T}} = \begin{pmatrix}
\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \hat{\mathbf{T}} = \begin{pmatrix}
(\hat{T}_{1} + \hat{T}_{2})/2 \\
(\hat{T}_{1} + \hat{T}_{2})/2 \\
\hat{T}_{3} \\
0 \\
0 \\
0
\end{pmatrix}.$$
(120)

The projection $\hat{\mathbf{T}}_0$ can be identified as the part of $\hat{\mathbf{T}}$ which displays hexagonal (or transversely isotropic) symmetry about the axis \mathbf{e}_3 . To be more precise, if we denote the projection $\widehat{\mathbf{M}}_0 \hat{\mathbf{T}}$ as $\hat{\mathbf{T}}_{\text{Hex}}$, then $\hat{\mathbf{T}}_{\text{Hex}}$ is invariant under the action of the symmetry group of rotations about \mathbf{p} . It may also be shown that of all tensors with hexagonal symmetry $\hat{\mathbf{T}}_{\text{Hex}}$ is the closest to $\hat{\mathbf{T}}$ using a Euclidean norm for distance. Similarly,

$$\hat{\mathbf{T}}_1 = \widehat{\mathbf{M}}_1 \hat{\mathbf{T}} = (0, 0, 0, \hat{T}_4, \hat{T}_5, 0)^t, \qquad \hat{\mathbf{T}}_2 = \widehat{\mathbf{M}}_2 \hat{\mathbf{T}} = (\frac{1}{2}(\hat{T}_1 - \hat{T}_2), \frac{1}{2}(\hat{T}_2 - \hat{T}_1), 0, 0, 0, \hat{T}_6)^t, (121)$$

and using eqs. (82) and (121),

$$\hat{\mathbf{R}}_1 = (0, 0, 0, \hat{T}_5, -\hat{T}_4, 0)^t, \qquad \hat{\mathbf{R}}_2 = (-\frac{1}{\sqrt{2}}\hat{T}_6, \frac{1}{\sqrt{2}}\hat{T}_6, 0, 0, 0, \frac{1}{\sqrt{2}}(\hat{T}_1 - \hat{T}_2))^t.$$
 (122)

It can be checked that under rotation, we have

$$\hat{\mathbf{Q}}\hat{\mathbf{T}}_0 = \hat{\mathbf{T}}_0, \qquad \hat{\mathbf{Q}}\hat{\mathbf{T}}_j = \cos j\theta \hat{\mathbf{T}}_j + \sin j\theta \hat{\mathbf{R}}_j, \qquad \hat{\mathbf{Q}}\hat{\mathbf{R}}_j = \cos j\theta \hat{\mathbf{R}}_j - \sin j\theta \hat{\mathbf{T}}_j, \quad j = 1, 2. \quad (123)$$

Thus, the singleton $\hat{\mathbf{T}}_0$ and pairs $(\hat{\mathbf{T}}_1, \hat{\mathbf{R}}_1)$ and $(\hat{\mathbf{T}}_2, \hat{\mathbf{R}}_2)$ form closed groups under the action of the rotation.

6.2.3 Elastic moduli, n=4

The 5-dimensional null space of $\tilde{\mathbf{P}}$ is equal to the set of base elasticity tensors for transverse isotropy (23; 8; 14). The projector follows from eqs. (106) and (107) as

$$\widetilde{\mathbf{M}}_{0} \equiv \frac{1}{(4!)^{2}} (\widetilde{\mathbf{P}}^{2} + 1) (\widetilde{\mathbf{P}}^{2} + 4) (\widetilde{\mathbf{P}}^{2} + 9) (\widetilde{\mathbf{P}}^{2} + 16) = \sum_{x=a,b,c,d,e} \widetilde{\mathbf{v}}_{0x} \widetilde{\mathbf{v}}_{0x}.$$
(124)

This is equivalent to the 8-th order projection tensor P_{Hex} of eq. (68c) of Moakher and Norris (17), who use the base tensors suggested by Walpole (22). The latter representation is useful because Walpole's tensors have a nice algebraic structure, making tensor products simple. Alternatively, in the spirit of the 21×21 representation of elastic moduli, (124)₁ and (101) yield

$$\widetilde{M}_{0}(\mathbf{e}_{3}) = \begin{pmatrix} M_{\text{Hex}} & \mathbf{0}_{9 \times 12} \\ \mathbf{0}_{12 \times 9} & \mathbf{0}_{12 \times 12} \end{pmatrix}, \qquad M_{\text{Hex}} = \begin{pmatrix} \frac{3}{8} & \frac{3}{8} & 0 & 0 & 0 & \frac{1}{4\sqrt{2}} & 0 & 0 & \frac{1}{4} \\ \frac{3}{8} & \frac{3}{8} & 0 & 0 & 0 & \frac{1}{4\sqrt{2}} & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{1}{4\sqrt{2}} & \frac{1}{4\sqrt{2}} & 0 & 0 & 0 & \frac{3}{4} & 0 & 0 & -\frac{1}{2\sqrt{2}} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & -\frac{1}{2\sqrt{2}} & 0 & 0 & \frac{1}{2} \end{pmatrix}.$$

$$(125)$$

The projection \widetilde{M}_0 of (125) is identical to the matrix derived by Browaeys and Chevrot (6) for projection of elastic moduli onto hexagonal symmetry. Specifically, the 9×9 matrix M_{Hex} is exactly $\mathbf{M}^{(4)}$ of Browaeys and Chevrot (see Appendix A of (6)). Hence, \widetilde{M}_0 of (125) provides an algorithm for projection onto hexagonal symmetry for arbitrary axis \mathbf{p} .

The subspace of \widetilde{T}_0 is 5-dimensional, while the subspaces $(\widetilde{T}_1, \widetilde{R}_1)$, $(\widetilde{T}_2, \widetilde{R}_2)$, $(\widetilde{T}_3, \widetilde{R}_3)$ and $(\widetilde{T}_4, \widetilde{R}_4)$ have dimensions 6, 6, 2 and 2, respectively. These may be evaluated for arbitrary axis of rotation \mathbf{p} using the prescription in eqs. (28c) and (113).

A. Appendix: A recursion

Equation (37) provides an expansion in terms of basic trigonometric functions. An alternative recursive procedure is derived here. Consider the expression (37) written

$$e^B = f_m(B), (A.1)$$

where the function $f_m(B)$ is a finite series defined by the m distinct pairs of non-zero eigenvalues of B. Suppose the set of eigenvalues is augmented by one more pair, $\pm ic_{m+1}$, with the others unchanged. Then the sums and products in (37) change to reflect the new eigenvalues,

$$e^{B} = f_{m+1}(B) = I + \sum_{j=1}^{m+1} \left[c_j \sin c_j B + (1 - \cos c_j) B^2 \right] c_j^{-2} \prod_{\substack{k=1\\k \neq j}}^{m+1} \left(\frac{B^2 + c_k^2}{c_k^2 - c_j^2} \right).$$
 (A.2)

The effect of the two additional eigenvalues can be isolated using the identity

$$\frac{B^2 + c_{m+1}^2}{c_{m+1}^2 - c_i^2} = 1 + \frac{B^2 + c_j^2}{c_{m+1}^2 - c_i^2},\tag{A.3}$$

to give

$$f_{m+1} = f_m + \left(\sum_{j=1}^{m+1} \frac{c_j \sin c_j B + (1 - \cos c_j) B^2}{c_j^2 \prod_{\substack{l=1 \ l \neq j}}^{m+1} (c_l^2 - c_j^2)}\right) \prod_{k=1}^m (B^2 + c_k^2).$$
(A.4)

This defines the sequence, starting with $f_0 = I$.

Applying this to the rotation $\exp(\theta \mathbb{P})$, and noting that the eigenvalues of the skew symmetric tensor \mathbb{P} correspond to $c_j = j\theta$, gives

$$P_{2n+2}(\theta,x) = P_{2n}(\theta,x) + \left(\sum_{j=1}^{n+1} \frac{j\sin j\theta \, x + (1-\cos j\theta) \, x^2}{j^2 \prod_{\substack{l=1\\l\neq j}}^{n+1} (l^2 - j^2)}\right) \prod_{k=1}^{n} (x^2 + k^2) \,. \tag{A.5}$$

The sum over trigonometric functions may be simplified using formulas for $\sin n\theta$ and $\cos n\theta$ in terms of $\cos \theta/2$ powers of $\sin \theta/2$ in Section 1.33 of Gradshteyn et al. (10). Thus,

$$\sum_{j=1}^{n+1} \frac{\sin j\theta}{\int_{\substack{l=1\\l\neq j}}^{n+1} (l^2 - j^2)} = \frac{(2\sin\frac{\theta}{2})^{2n+1}}{(2n+1)!} \cos\frac{\theta}{2},\tag{A.6}$$

$$\sum_{j=1}^{n+1} \frac{1 - \cos j\theta}{j^2 \prod_{\substack{l=1\\l \neq j}}^{n+1} (l^2 - j^2)} = \frac{(2\sin\frac{\theta}{2})^{2n+1}}{(2n+1)!} \frac{\sin\frac{\theta}{2}}{n+1},\tag{A.7}$$

and hence,

$$P_{2n+2}(\theta,x) = P_{2n}(\theta,x) + \frac{(2\sin\frac{\theta}{2})^{2n+1}}{(2n+1)!} \left(\cos\frac{\theta}{2}x + (n+1)^{-1}\sin\frac{\theta}{2}x^2\right) \prod_{k=1}^{n} (x^2 + k^2), \tag{A.8}$$

from which the expression (18b) follows.

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 $2 p_2$ $2 p_3$ $-2 p_1$ $2 p_1$ $-2 p_2$ $-\sqrt{2}p_2$ $-\sqrt{2}p_1$ $\sqrt{2}p_3$ $\sqrt{2}p_1$ $\sqrt{2}p_1$ $-\sqrt{2}p_3$ $-\sqrt{2}p_{2}$ $\sqrt{2}p_2$ $\sqrt{2}p_2$ $-\sqrt{2}p_3$ $-\sqrt{2}p_1$ $\sqrt{2}p_3$ $\sqrt{2}p_3$ $-2 p_1$ $2 p_1$ $\sqrt{2}p_1$ $-\sqrt{2}p_3$ $-2 p_2$ $2 p_2$ $-\sqrt{2}p_1$ $\sqrt{2}p_2$ $-2 p_{3}$ $-\sqrt{2}p_1$ $-\sqrt{2}p_3$ $\sqrt{2}p_1$ $\sqrt{2}p_2$ $-p_2$ $\sqrt{2}p_2$ $\sqrt{2}p_3$ $-\sqrt{2}p_2$ $-\sqrt{2}p_1$ p_1 $-p_3$ $-\sqrt{2}p_3$ $\sqrt{2}p_3$ $-\sqrt{2}p_2$ $\sqrt{2}p_1$ $-p_{1}$ $\sqrt{2}p_1$ $-2 p_1$ $-\sqrt{2}p_2$ $2 p_1$ $-\sqrt{2}p_3$ $-2\,p_2$ $\sqrt{2}p_2$ $2 p_2$ $-p_3$ $-\sqrt{2}p_1$ $\sqrt{2}p_3$ $2 p_3$ $-2 p_{3}$ $-\sqrt{2}p_1$ $\sqrt{2}p_3$ $2 p_1$ $-2 p_1$ $-\sqrt{2}p_2$ $-2 p_{2}$ $\sqrt{2}p_1$ $2p_2$ p_1 $-\sqrt{2}p_3$ $-2 p_{3}$ $\sqrt{2}p_2$ $2 p_3$ p_2 $-p_1$ $\sqrt{2}p_1$ $-\sqrt{2}p_1$ $-\sqrt{2}p_2$ $\sqrt{2}p_2$ $\sqrt{2}p_3$ p_2 $\sqrt{2}p_2$ $-\sqrt{2}p_2$ $\sqrt{2}p_3$ $-\sqrt{2}p_1$ $\sqrt{2}p_1$ $-\sqrt{2}p_3$ p_3 $-p_1$ $-\sqrt{2}p_3$ $\sqrt{2}p_3$ $-\sqrt{2}p_2$ $\sqrt{2}p_1$ $\sqrt{2}p_2$ $-\sqrt{2}p_1$ $-p_2$

Table 1. The matrix $\widetilde{\mathbf{P}}(\mathbf{p}) \in so(21)$ for 4th order elasticity tensors represented as 21-vectors. The rotation $\widetilde{\mathbf{Q}} = \exp(\theta \widetilde{\mathbf{P}})$ is given by the 8-th order polynomial $\widetilde{\mathbf{Q}} = P_8(\theta, \widetilde{\mathbf{P}})$ of eq. (20).